```
=> fil reg
FILE 'REGISTRY' ENTERED AT 18:12:30 ON 05 OCT 2007
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STRUCTURE FILE UPDATES:    4 OCT 2007  HIGHEST RN 949197-90-4
DICTIONARY FILE UPDATES:   4 OCT 2007  HIGHEST RN 949197-90-4

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> d que stat l20
L4                SCR 2040
L6                STR
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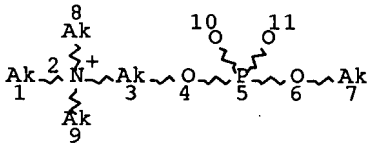


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NODE ATTRIBUTES:
CHARGE  IS *+     AT   2
CONNECT IS E1  RC AT   1
CONNECT IS E2  RC AT   3
CONNECT IS E1  RC AT   8
CONNECT IS E1  RC AT   9
DEFAULT MLEVEL IS ATOM
GGCAT   IS SAT  AT   1
GGCAT   IS SAT  AT   3
GGCAT   IS SAT  AT   7
GGCAT   IS SAT  AT   8
GGCAT   IS SAT  AT   9
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  11

STEREO ATTRIBUTES: NONE
L8        10632 SEA FILE=REGISTRY SSS FUL L6 AND L4
L16             SCR 2043 OR 1838
L18             STR
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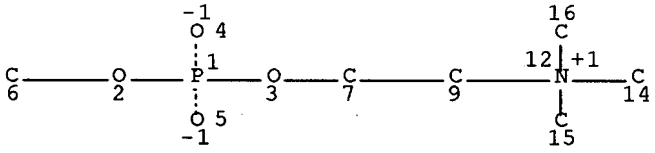


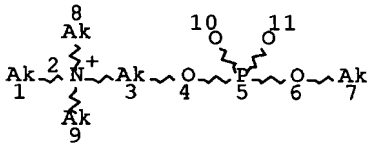
NODE ATTRIBUTES:
CHARGE IS E-1 AT 4
CHARGE IS E-1 AT 5
CHARGE IS E+1 AT 12
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE
L20 6136 SEA FILE=REGISTRY SUB=L8 SSS FUL L18 NOT L16

100.0% PROCESSED 6502 ITERATIONS 6136 ANSWERS
SEARCH TIME: 00.00.01

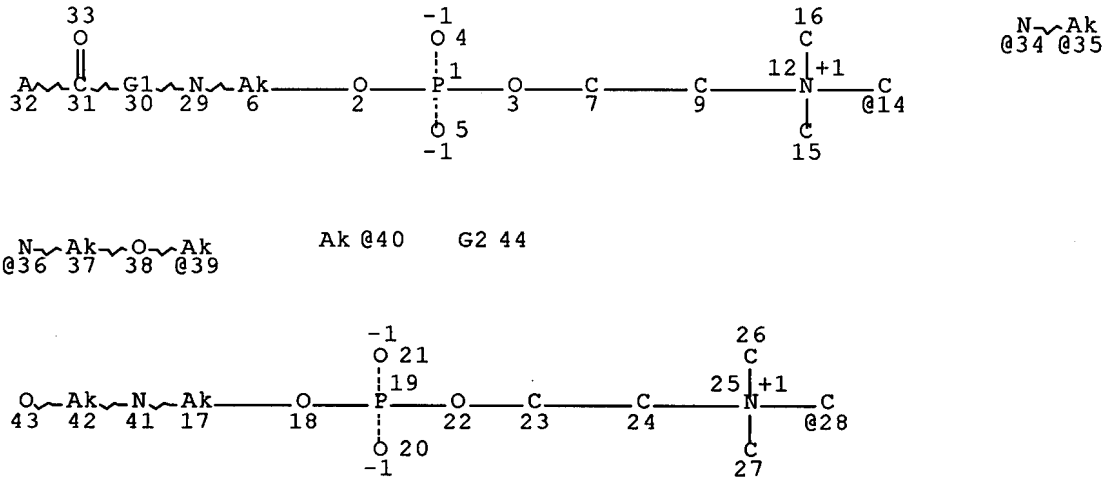
=> d que stat l41
L4 SCR 2040
L6 STR



NODE ATTRIBUTES:
CHARGE IS *+ AT 2
CONNECT IS E1 RC AT 1
CONNECT IS E2 RC AT 3
CONNECT IS E1 RC AT 8
CONNECT IS E1 RC AT 9
DEFAULT MLEVEL IS ATOM
GGCAT IS SAT AT 1
GGCAT IS SAT AT 3
GGCAT IS SAT AT 7
GGCAT IS SAT AT 8
GGCAT IS SAT AT 9
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE
L8 10632 SEA FILE=REGISTRY SSS FUL L6 AND L4
L39 STR



Ak @40 G2 44

VAR G1=34-31 35-29/40/36-31 39-29
VAR G2=14/28
NODE ATTRIBUTES:
CHARGE IS E-1 AT 4
CHARGE IS E-1 AT 5
CHARGE IS E+1 AT 12
CHARGE IS E-1 AT 20
CHARGE IS E-1 AT 21
CHARGE IS E+1 AT 25
CONNECT IS E2 RC AT 6
CONNECT IS E2 RC AT 17
CONNECT IS E2 RC AT 35
CONNECT IS E2 RC AT 37
CONNECT IS E2 RC AT 39
CONNECT IS E2 RC AT 40
CONNECT IS E2 RC AT 42
DEFAULT MLEVEL IS ATOM
GGCAT IS SAT AT 17
GGCAT IS SAT AT 35
GGCAT IS SAT AT 37
GGCAT IS SAT AT 39
GGCAT IS SAT AT 40
GGCAT IS SAT AT 42
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 40

STEREO ATTRIBUTES: NONE
L41 74 SEA FILE=REGISTRY SUB=L8 SSS FUL L39

100.0% PROCESSED 9899 ITERATIONS 74 ANSWERS
SEARCH TIME: 00.00.01

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L1             1 SEA ABB=ON  PLU=ON  US2005222405/PN
                 SEL RN

     FILE 'REGISTRY' ENTERED AT 16:24:45 ON 05 OCT 2007
L2            15 SEA ABB=ON  PLU=ON  (53571-87-2/BI OR 9044-05-7/BI OR
                 107-15-3/BI OR 143-07-7/BI OR 28319-77-9/BI OR 335-67-1/B
                 I OR 57-11-4/BI OR 612845-13-3/BI OR 612845-14-4/BI OR
                 612845-15-5/BI OR 7790-28-5/BI OR 79-11-8/BI OR 9000-11-7
                 /BI OR 9004-54-0/BI OR 9004-61-9/BI)
                 D SCA

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L3               STR

     FILE 'REGISTRY' ENTERED AT 16:55:53 ON 05 OCT 2007
L4               SCR 2040
L5             8 SEA SSS SAM L3 AND L4
L6               STR L3
L7            50 SEA SSS SAM L6 AND L4
L8         10632 SEA SSS FUL L6 AND L4
                 SAV L8 BLA771/A
L9             1 SEA ABB=ON  PLU=ON  L2 AND L8
L10              STR 28319-77-9
L11              STR L6
L12           50 SEA SUB=L8 SSS SAM L11
L13              SCR 2043
L14           50 SEA SUB=L8 SSS SAM L11 NOT L13

     FILE 'LREGISTRY' ENTERED AT 17:06:49 ON 05 OCT 2007
L15              STR L11
L16              SCR 2043 OR 1838

     FILE 'REGISTRY' ENTERED AT 17:09:44 ON 05 OCT 2007
L17            3 SEA SUB=L8 SSS SAM L15 NOT L16
                 D SCA

     FILE 'LREGISTRY' ENTERED AT 17:21:17 ON 05 OCT 2007
L18              STR L10

     FILE 'REGISTRY' ENTERED AT 17:22:08 ON 05 OCT 2007
L19           50 SEA SUB=L8 SSS SAM L18 NOT L16
L20         6136 SEA SUB=L8 SSS FUL L18 NOT L16
L21            1 SEA ABB=ON  PLU=ON  L2 AND L20
                 SAV L20 BLA771S1/A
L22            1 SEA ABB=ON  PLU=ON  56-87-1/RN

     FILE 'HCAPLUS' ENTERED AT 17:30:46 ON 05 OCT 2007
L23          839 SEA ABB=ON  PLU=ON  L20/D

     FILE 'REGISTRY' ENTERED AT 17:36:56 ON 05 OCT 2007
L24            1 SEA ABB=ON  PLU=ON  "2,4-DIAMINOBUTANOIC ACID"/CN
                 D SCA
L25            1 SEA ABB=ON  PLU=ON  305-62-4/RN
L26           21 SEA ABB=ON  PLU=ON  305-62-4/CRN
L27         2434 SEA ABB=ON  PLU=ON  56-87-1/CRN

     FILE 'HCAPLUS' ENTERED AT 17:43:50 ON 05 OCT 2007
L28        52375 SEA ABB=ON  PLU=ON  L22 OR L25
L29        13898 SEA ABB=ON  PLU=ON  L26 OR L27
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L30          10 SEA ABB=ON  PLU=ON  L23 AND L28
L31           9 SEA ABB=ON  PLU=ON  L23 AND L29
L32             QUE ABB=ON  PLU=ON  ?POLYSACCHARIDE? OR SUGAR?
L33          40 SEA ABB=ON  PLU=ON  L23 AND L32
L34         137 SEA ABB=ON  PLU=ON  L20(L)L32
L35           0 SEA ABB=ON  PLU=ON  L34 AND L28
L36           2 SEA ABB=ON  PLU=ON  L34 AND L29

     FILE 'LREGISTRY' ENTERED AT 17:46:34 ON 05 OCT 2007
L37             STR L18

     FILE 'REGISTRY' ENTERED AT 18:02:26 ON 05 OCT 2007
L38          21 SEA SUB=L8 SSS SAM L37
L39             STR L37
L40           4 SEA SUB=L8 SSS SAM L39
L41          74 SEA SUB=L8 SSS FUL L39
                SAV L41 BLA771S2/A

     FILE 'HCAPLUS' ENTERED AT 18:06:07 ON 05 OCT 2007
L42          43 SEA ABB=ON  PLU=ON  L41
L43           1 SEA ABB=ON  PLU=ON  L42 AND L32
L44           0 SEA ABB=ON  PLU=ON  L41(L)L32
L45           2 SEA ABB=ON  PLU=ON  L33 AND L28
L46           3 SEA ABB=ON  PLU=ON  L33 AND L29
L47           6 SEA ABB=ON  PLU=ON  L36 OR L45 OR L46
L48          42 SEA ABB=ON  PLU=ON  L42 NOT (L43 OR L47)
L49          34 SEA ABB=ON  PLU=ON  L48 AND (PY<=2003 OR PRY<=2003 OR
                AY<=2003)



=> fil hcap
FILE 'HCAPLUS' ENTERED AT 18:12:43 ON 05 OCT 2007
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FILE LAST UPDATED: 4 Oct 2007  (20071004/ED)

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 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=> d 143 ibib abs hitstr hitind

L43  ANSWER 1 OF 1  HCAPLUS  COPYRIGHT 2007 ACS on STN
```

ACCESSION NUMBER: 1989:121101 HCAPLUS Full-text
DOCUMENT NUMBER: 110:121101
TITLE: Skin conditioners containing alkanolamides and amino alcohols
INVENTOR(S): Yano, Shinji; Kawamata, Akira; Minematsu, Yoshihiro; Akazaki, Shuichi; Zama, Mitsuko; Imokawa, Genji; Takaishi, Naotake; Ohtomo, Tsuyoshi; Komori, Takashi
PATENT ASSIGNEE(S): Kao Corp., Japan
SOURCE: Eur. Pat. Appl., 53 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 282816	A2	19880921	EP 1988-103177	19880302
EP 282816	A3	19910403		
EP 282816	B1	19930915		
R: DE, ES, FR, GB, IT				
JP 63216812	A	19880909	JP 1987-51276	19870306
JP 06092293	B	19941116		
JP 63218609	A	19880912	JP 1987-53769	19870309
JP 06092294	B	19941116		
JP 63222107	A	19880916	JP 1987-56049	19870311
JP 06092295	B	19941116		
JP 63227513	A	19880921	JP 1987-60718	19870316
JP 06092296	B	19941116		
JP 63227514	A	19880921	JP 1987-60719	19870316
JP 06092297	B	19941116		
JP 63297309	A	19881205	JP 1987-132054	19870528
JP 06092298	B	19941116		
JP 01009905	A	19890113	JP 1987-163682	19870630
JP 06069930	B	19940907		
JP 01009906	A	19890113	JP 1987-163683	19870630
JP 06069931	B	19940907		
JP 01009907	A	19890113	JP 1987-163685	19870630

JP 06069932	B	19940907		
EP 534286	A1	19930331	EP 1992-115766	198803 02
EP 534286	B1	19950802		
R: DE, ES, FR, GB, IT				
ES 2077948	T3	19951201	ES 1992-115766	198803 02
US 4985547	A	19910115	US 1988-163835	198803 03
JP 01079195	A	19890324	JP 1988-133426	198805 31
US 5028416	A	19910702	US 1990-546276	199006 29
US 5071971	A	19911210	US 1990-584739	199009 19

PRIORITY APPLN. INFO.:	JP 1987-51276	A	198703 06
	JP 1987-53769	A	198703 09
	JP 1987-56049	A	198703 11
	JP 1987-60718	A	198703 16
	JP 1987-60719	A	198703 16
	JP 1987-132054	A	198705 28
	JP 1987-138727	A	198706 02
	JP 1987-163682	A	198706 30
	JP 1987-163683	A	198706 30
	JP 1987-163685	A	198706 30

US 1988-163835 A3
198803
03

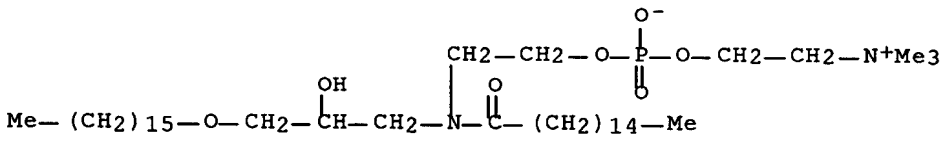
OTHER SOURCE(S): MARPAT 110:121101

AB Skin-care cosmetics contain fatty alkanolamides or amino alcs. The alkanolamides comprise R1CONACH2B [I; R1 = aliphatic hydrocarbyl; A = (CH2)1H (1 = 3-6); CX1X2CHX3OH (X1-X3 = H, alkyl, hydroxyalkyl); (CH2CH2O)mH (m = 1, 2); CHR2CO2Y (Y = H, alkali metal; R2 = H, Me, PhCH2, Me2CH, Me2CHCH2, EtMeCHCH2, HOCH2, MeCH(OH), MeSCH2CH2, YO2CCH2, YO2CCH2CH2, 4-HOC6H4CH2, imidazol-4-ylmethyl, indol-3-ylmethyl, CH2CH2OR3 where R3 = **sugar** residue, P(O)(O-)OCH2CH2N+Z1Z2Z3 where Z1-Z3 = H, alkyl, aralkyl); B = CH(OR4)CH2OR5 (R4 = H, **sugar** residue, P(O)(O-)CH2CH2N+Z1Z2Z3, (CH2CH2O)nH where n = ≥1; R5 = aliphatic hydrocarbyl, CHOHR5; with the proviso that X1-X3 and R4 may not be H the same time]. The amino alcs. comprise R6OCH2CH(OH)CH2NR8CH2CH(OH)CH2OR7 (II; R6, R7 = aliphatic hydrocarbyl; R8 = CH2CH2OH, CH2CO2H, Ac). Several I are prepared The cosmetics presented here enhance the moisture-retaining ability of the skin and relieve roughness of the skin. II were applied to rough skin for 2 wk and skin roughness was scored from 0 (no roughness) to 5 (severely rough skin); the score was 0.9 for II (R6 = R7 = n-C18H37, R6 = CH2CH2OH) (III) alone, 0.1-0.7 for III when incorporated in a formulations. An emulsion type cosmetic foundation contained III 3.0, stearic acid 5.0, cetostearyl alc. 1.0, jojoba oil 15.0, glycerol monostearate 2.0, propylene glycol monolaurate 3.0, propylene glycol 4.0, triethanolamine 1.2, methylparaben 0.3, perfume 0.1, TiO2 8.0, talc 4.0, Fe oxide 0.5, and H2O to 100% by weight

IT **119093-59-3 119093-61-7 119093-63-9**
119093-65-1 119135-32-9
RL: BIOL (Biological study)
(skin conditioning cosmetics containing)

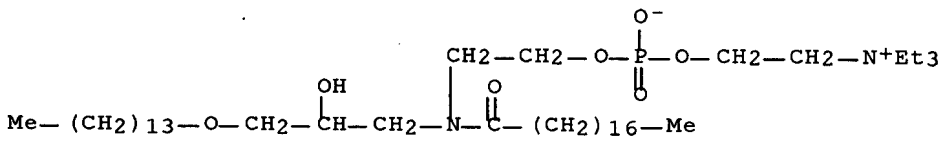
RN 119093-59-3 HCAPLUS

CN 3,5,12-Trioxa-8-aza-4-phosphaoctacosan-1-aminium, 4,10-dihydroxy-N,N,N-trimethyl-8-(1-oxohexadecyl)-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



RN 119093-61-7 HCAPLUS

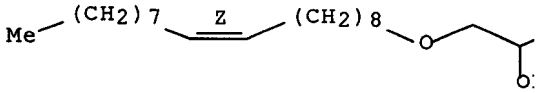
CN 3,5,12-Trioxa-8-aza-4-phosphahexacosan-1-aminium, N,N,N-triethyl-4,10-dihydroxy-8-(1-oxooctadecyl)-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



RN 119093-63-9 HCAPLUS

CN 3,5,12-Trioxa-8-aza-4-phospha
4,10-dihydroxy-N,N,N-trimethy
4-oxide, (Z)- (9CI) (CA INDE

Double bond geometry as shown.



RN 119093-65-1 HCAPLUS
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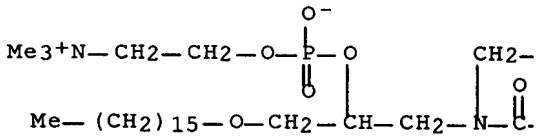
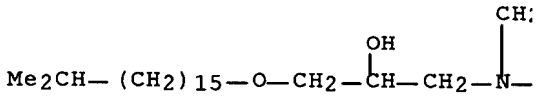
6-[(hexadecyloxy)methyl]-4,12
(1-oxohexadecyl)-, bis(inner
NAME)



RN 119135-32-9 HCAPLUS
CN 3,5,12-Trioxa-8-aza-4-phospha
4,10-dihydroxy-N,N,N,28-tetra
inner salt, 4-oxide (9CI) (C



IC ICM A61K007-48
CC 62-4 (Essential Oils and Cosm
Section cross-reference(s): 2
IT 65212-53-5 119093-57-1 11
119093-60-6 **119093-61-7** 119
119093-64-0 **119093-65-1** 119
119093-68-4 119093-69-5 1
119093-73-1 119093-74-2 1
119093-78-6 119093-79-7 1
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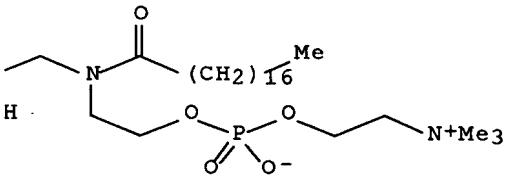
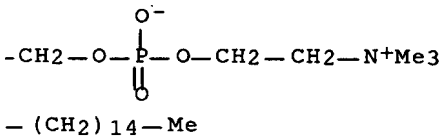
19093-95-7 119093-96-8 119093-97-9
19094-00-7 119094-01-8 119094-02-9
19094-05-2 119094-06-3 119094-07-4
135-32-9 119135-33-0

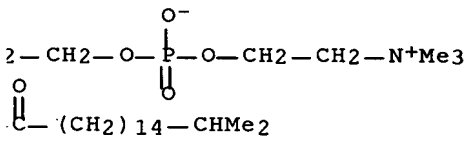
triacont-21-en-1-aminium,
1-8-(1-oxooctadecyl)-, inner salt,
X NAME)



-diphosphapentadecane-1,15-diaminium,
-dihydroxy-N,N,N,N',N',N'-hexamethyl-8-
salt), 4,12-dioxide (9CI) (CA INDEX



nonacosan-1-aminium,
methyl-8-(16-methyl-1-oxoheptadecyl)-,
A INDEX NAME)



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093-62-8 **119093-63-9**
093-66-2 119093-67-3
19093-70-8 119093-71-9 119093-72-0
19093-75-3 119093-76-4 119093-77-5

119135-34-1 119135-35-2 119135-36-3
RL: BIOL (Biological study)
(skin conditioning cosmetics containing)

=> d l47 ibib abs hitstr hitind 1-6

L47 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:1223834 HCAPLUS Full-text
DOCUMENT NUMBER: 143:476388
TITLE: Therapeutic vaccine comprising P-170 glycoprotein peptides conjugated with phospholipid for inhibiting multidrug resistance in treatment of cancers
INVENTOR(S): Tosi, Pierre-Francois; Madoulet, Claudie; Nicolau, Claude Yves; Hickman, David T.
PATENT ASSIGNEE(S): Fr.
SOURCE: U.S. Pat. Appl. Publ., 30 pp., Cont.-in-part of U.S. Ser. No. 902,276.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005255561	A1	20051117	US 2005-59633	200502 16
FR 2857875	A1	20050128	FR 2003-9188	200307 25
WO 2005014036	A1	20050217	WO 2004-EP8330	200407 25
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2005175615	A1	20050811	US 2004-902276	200407 30
US 2006233758	A1	20061019	US 2005-274885	200511 16
PRIORITY APPLN. INFO.:			FR 2003-9188 A	200307 25
			WO 2004-EP8330 A1	

200407
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US 2004-902276 A2
200407
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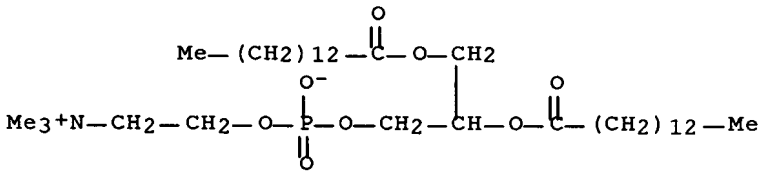
US 2005-59633 A2
200502
16

AB The invention relates to conjugates comprising all or part of the amino acid sequences of at least one peptide derived from an extracellular loop of the P-170 protein. The peptide may be covalently attached to spacers which may be polyethyleneglycol (PEG), polyglycine, polylysine or any polymer chain suitable for human use and is coupled at its free end to a phospholipids, e.g., phosphatidylethanolamine or any other chemical suitable phospholipid. The p-170 peptide-phospholipid conjugates are used to inhibit multidrug resistance and in combination with an antitumor treatment. The invention also includes diagnostic kit comprising labeled monoclonal antibody for detecting P-170 glycoprotein in biol. sample or solid tumor expressing MDR1 gene encoding human P-glycoprotein.

IT **18656-38-7D**, Dimyristoylphosphatidylcholine, conjugates
25104-18-1D, Poly-L-lysine, conjugates
RL: BSU (Biological study, unclassified); DGN (Diagnostic use); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(therapeutic vaccine comprising P-170 glycoprotein peptides conjugated with phospholipid for inhibiting multidrug resistance in treatment of cancers)

RN 18656-38-7 HCAPLUS
CN 3,5,9-Trioxa-4-phosphatricosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-10-oxo-7-[(1-oxotetradecyl)oxy]-, inner salt, 4-oxide (CA INDEX NAME)

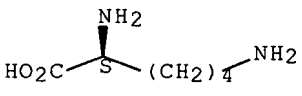


RN 25104-18-1 HCAPLUS
CN L-Lysine, homopolymer (CA INDEX NAME)

CM 1

CRN 56-87-1
CMF C6 H14 N2 O2

Absolute stereochemistry.



IC ICM C07H021-04
ICS C12P021-06; C07K014-705
INCL 435069700; 435320100; 435325000; 530395000; 536023500
CC 15-2 (Immunochemistry)
Section cross-reference(s): 1, 9, 63
IT Antibodies and Immunoglobulins
Antigens
Enzymes, biological studies
Fatty acids, biological studies
Lipid A
Phosphatidylethanolamines, biological studies
Phospholipids, biological studies
Polymers, biological studies
Polyoxyalkylenes, biological studies
Polysaccharides, biological studies
Radionuclides, biological studies
RL: BSU (Biological study, unclassified); DGN (Diagnostic use); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(therapeutic vaccine comprising P-170 glycoprotein peptides conjugated with phospholipid for inhibiting multidrug resistance in treatment of cancers)
IT 57-88-5D, Cholesterol, conjugates 2462-63-7D, Dioleoyl phosphatidylethanolamine, conjugates 4537-76-2, Distearoylphosphatidylethanolamine 4539-70-2, Distearoylphosphatidylcholine 5681-36-7D, Dipalmitoyl phosphatidylethanolamine, conjugates **18656-38-7D**, Dimyristoylphosphatidylcholine, conjugates 20255-95-2D, Dimyristoyl phosphatidylethanolamine, conjugates **25104-18-1D**, Poly-L-lysine, conjugates 25322-68-3D, Polyethylene glycol, conjugates 25322-69-4D, Polypropylene glycol, conjugates 25513-46-6D, Poly-L-glutamic acid, conjugates 25718-94-9D, Polyglycine, conjugates 61361-72-6D, Dimyristoylphosphatidylglycerol, conjugates
RL: BSU (Biological study, unclassified); DGN (Diagnostic use); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(therapeutic vaccine comprising P-170 glycoprotein peptides conjugated with phospholipid for inhibiting multidrug resistance in treatment of cancers)

L47 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:983946 HCAPLUS Full-text
DOCUMENT NUMBER: 143:284695
TITLE: Supramolecular constructs comprising antigenic epitopes for vaccines against neurological, hyperproliferative and infectious diseases
INVENTOR(S): Nicolau, Yves Claude; Greferath, Ruth; Hickman, David
PATENT ASSIGNEE(S): AC Immune S. A., Switz.
SOURCE: PCT Int. Appl., 60 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005081872	A2	20050909	WO 2005-US5285	200502

22

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2004242845	A1	20041202	US 2004-783975	200402 20
US 2006073158	A1	20060406	US 2004-958211	200410 04
AU 2005216100	A1	20050909	AU 2005-216100	200502 22
CA 2556479	A1	20050909	CA 2005-2556479	200502 22
EP 1763364	A2	20070321	EP 2005-723323	200502 22

R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU

JP 2007527870	T	20071004	JP 2006-554250	200502 22

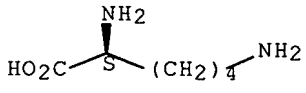
PRIORITY APPLN. INFO.:	US 2004-783975	A	200402 20
	US 2004-958211	A	200410 04
	US 2003-449573P	P	200302 21
	WO 2005-US5285	W	200502 22

AB The present invention comprises novel compns. and methods for eliciting high immune responses, of great specificity yielding conformationally sensitive antibodies. These antibodies recognize specific epitopes on a wide variety of antigens including but not limited to, amyloid protein, prion protein or P170 glycoprotein. The novel compns. of the invention comprise supramol. antigenic constructs generally comprising a peptide sequence, covalently attached to pegylated lysine resulting in modified and enhanced peptide presentation. The unique modification methodol. of the present invention is applicable to a variety of peptides and can ultimately be employed in therapeutic formulations and vaccines for diseases and disorders such as Alzheimer's disease.

IT **56-87-1D**, L-Lysine, pegylated conjugates **18194-24-6D**
, Dimyristoyl phosphatidylcholine, conjugates **68737-67-7D**,
conjugates
RL: BSU (Biological study, unclassified); THU (Therapeutic use);
BIOL (Biological study); USES (Uses)
(supramol. constructs comprising antigenic epitopes for vaccines
against neurol., hyperproliferative and infectious diseases)

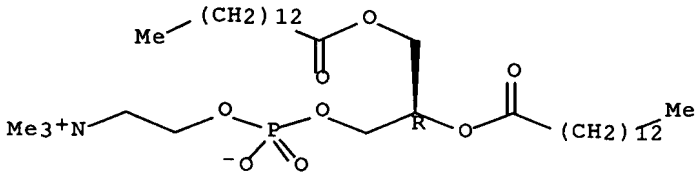
RN 56-87-1 HCAPLUS
CN L-Lysine (CA INDEX NAME)

Absolute stereochemistry.



RN 18194-24-6 HCAPLUS
CN 3,5,9-Trioxa-4-phosphatricosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-10-oxo-7-[(1-oxotetradecyl)oxy]-, inner salt, 4-oxide, (7R)- (CA INDEX NAME)

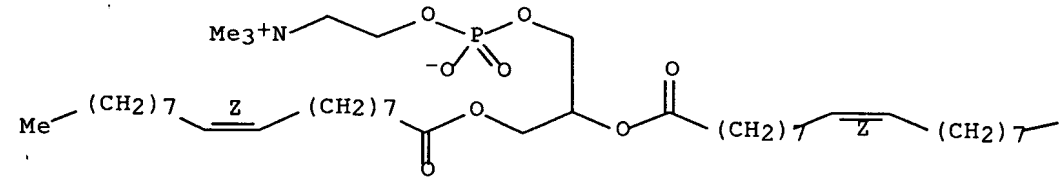
Absolute stereochemistry.



RN 68737-67-7 HCAPLUS
CN 3,5,9-Trioxa-4-phosphaheptacos-18-en-1-aminium, 4-hydroxy-N,N,N-trimethyl-10-oxo-7-[[(9Z)-1-oxo-9-octadecen-1-yl]oxy]-, inner salt, 4-oxide, (18Z)- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

IC ICM A61K
CC 15-2 (Immunochemistry)
Section cross-reference(s): 3, 63
IT Polymers, biological studies
Polysaccharides, biological studies
RL: BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(conjugates; supramol. constructs comprising antigenic epitopes for vaccines against neurol., hyperproliferative and infectious diseases)
IT Peptides, biological studies
Polyamides, biological studies
Polyesters, biological studies
Polymers, biological studies
Polyoxyalkylenes, biological studies
Polysaccharides, biological studies
Polyurethanes, biological studies
RL: BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(supramol. constructs comprising antigenic epitopes for vaccines against neurol., hyperproliferative and infectious diseases)
IT **56-87-1D**, L-Lysine, pegylated conjugates 57-10-3D, Palmitic acid, conjugates 57-88-5D, Cholesterol, conjugates 1398-61-4D, Chitin, conjugates 2462-63-7D, Dioleoylphosphatidylethanolamine, ethoxylated amyloid peptide conjugate derivs. 9012-76-4D, Chitosan, conjugates **18194-24-6D**, Dimyristoyl phosphatidylcholine, conjugates 20255-95-2D, Dimyristoyl phosphatidylethanolamine, conjugates 21442-01-3D, N-(2-Hydroxy)propyl methacrylamide, polymer or copolymer and conjugates 25087-26-7D, Polymethacrylic acid, polymer or copolymer and conjugates 25249-06-3D, Polygalacturonic acid, conjugates 25322-68-3D, Polyethylene glycol, amyloid peptide conjugate derivs. 25718-94-9D, Polyglycine, conjugates 26023-30-3D, Poly[oxy(1-methyl-2-oxo-1,2-ethanediyl)], conjugates 26062-48-6D, Poly-L-histidine, conjugates 26100-51-6D, Polylactic acid, conjugates 61361-72-6D, Dimyristoyl phosphatidyl glycerol, conjugates **68737-67-7D**, conjugates
RL: BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(supramol. constructs comprising antigenic epitopes for vaccines against neurol., hyperproliferative and infectious diseases)

L47 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:732493 HCAPLUS Full-text
DOCUMENT NUMBER: 143:206398
TITLE: Conjugates of amino acids with drugs or with imaging agents for cancer therapy and diagnosis
INVENTOR(S): Gengrinovitch, Stela; Izakovich, Esther
PATENT ASSIGNEE(S): Biosight Ltd., Israel
SOURCE: PCT Int. Appl., 73 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 2005072061 A2 20050811 WO 2005-IL117 200502 02

WO 2005072061 A3 20060824

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, SM

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1718145 A2 20061108 EP 2005-703160 200502 02

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, BA, HR, IS, YU

US 2007072800 A1 20070329 US 2006-497511 200608 02

PRIORITY APPLN. INFO.: US 2004-540334P P 200402 02

WO 2005-IL117 W 200502 02

OTHER SOURCE(S): MARPAT 143:206398

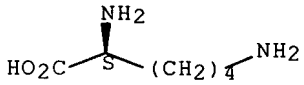
AB The invention discloses conjugates of a drug and an amino acid or an amino acid derivative or analog, pharmaceutical compns. comprising the conjugates and methods of use thereof. In particular, the invention discloses conjugates of antiproliferative drugs and asparagine and glutamine and analogs thereof as compns. for treatment of cancer, as well as conjugates of imaging agent carriers and amino acids for the diagnosis of tumors and metastases. Preparation of conjugates of the invention is described.

IT **56-87-1D**, L-Lysine, conjugates
RL: DGN (Diagnostic use); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(amino acid conjugates with drugs or with imaging agents for cancer therapy and diagnosis)

RN 56-87-1 HCAPLUS

CN L-Lysine (CA INDEX NAME)

Absolute stereochemistry.

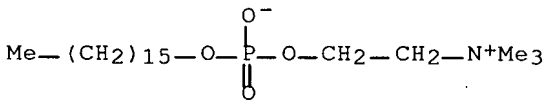


IT **58066-85-6D**, Miltefosine, amino acid conjugates
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL

(Biological study); USES (Uses)
(amino acid conjugates with drugs or with imaging agents for cancer therapy and diagnosis)

RN 58066-85-6 HCAPLUS

CN Ethanaminium, 2-[[(hexadecyloxy)hydroxyphosphinyl]oxy]-N,N,N-trimethyl-, inner salt (CA INDEX NAME)



IC ICM A61K

CC 1-6 (Pharmacology)
Section cross-reference(s): 9, 14, 34

IT Amino acids, biological studies
Polyanhydrides
Polymers, biological studies
Polyphosphazenes
Polysaccharides, biological studies
Polyurethanes, biological studies
Proteins
RL: DGN (Diagnostic use); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(conjugates; amino acid conjugates with drugs or with imaging agents for cancer therapy and diagnosis)

IT **Polysaccharides**, biological studies
RL: DGN (Diagnostic use); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(sulfated, conjugates; amino acid conjugates with drugs or with imaging agents for cancer therapy and diagnosis)

IT 51-35-4D, Hydroxyproline, conjugates 52-67-5D, Penicillamine, conjugates 52-90-4D, L-Cysteine, conjugates 56-45-1D, L-Serine, conjugates 56-84-8D, L-Aspartic acid, conjugates 56-85-9D, L-Glutamine, conjugates 56-86-0D, L-Glutamic acid, conjugates **56-87-1D**, L-Lysine, conjugates 60-18-4D, L-Tyrosine, conjugates 70-26-8D, Ornithine, conjugates 70-47-3D, L-Asparagine, conjugates 72-19-5D, L-Threonine, conjugates 73-22-3D, L-Tryptophan, conjugates 74-79-3D, L-Arginine, conjugates 110-16-7D, 2-Butenedioic acid (2Z)-, polymeric conjugates 300-39-0D, conjugates 372-75-8D, Citrulline, conjugates 672-15-1D, Homoserine, conjugates 943-80-6D, 4-Aminophenylalanine, conjugates 1190-49-4D, Homocitrulline, conjugates 2453-03-4D, Tri-methylenecarbonate, conjugates 3054-07-7D, α-Aminosuberic acid, conjugates 24980-41-4D, Poly(ε-caprolactone), conjugates 25248-42-4D, Poly[oxy(1-oxo-1,6-hexanediyl)], conjugates 25322-68-3D, Polyethylene glycol, conjugates 26009-03-0D, Polyglycolic acid, conjugates 26023-30-3D, Poly[oxy(1-methyl-2-oxo-1,2-ethanediyl)], conjugates 26100-51-6D, Poly-DL-lactic acid, conjugates 26124-68-5D, Polyglycolic acid, conjugates 26161-42-2D, conjugates 26811-96-1D, Poly-L-lactic acid, conjugates 29223-92-5D, conjugates 31621-87-1D, conjugates 49642-07-1D, Statine, conjugates 63531-84-0D, conjugates 75176-85-1D, 4-Aminophenylglycine, conjugates 862177-30-8D, conjugates 862177-33-1D, conjugates

RL: DGN (Diagnostic use); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(amino acid conjugates with drugs or with imaging agents for cancer therapy and diagnosis)

IT 50-18-0D, Cyclophosphamide, amino acid conjugates 50-44-2D, 6-Mercaptopurine, amino acid conjugates 50-76-0D, Dactinomycin, amino acid conjugates 50-91-9D, Floxuridine, amino acid conjugates 51-18-3D, Triethylenemelamine, amino acid conjugates 51-21-8D, Fluorouracil, amino acid conjugates 51-75-2D, Mechlorethamine, amino acid conjugates 51-79-6D, Urethan, amino acid conjugates 52-24-4D, Triethylenethiophosphoramide, amino acid conjugates 53-79-2D, Puromycin, amino acid conjugates 54-25-1D, 6-Azauridine, amino acid conjugates 54-91-1D, Pipobroman, amino acid conjugates 55-98-1D, Busulfan, amino acid conjugates 57-22-7D, Vincristine, amino acid conjugates 59-05-2D, Methotrexate, amino acid conjugates 66-75-1D, Uracil mustard, amino acid conjugates 68-76-8D, Triaziquone, amino acid conjugates 69-33-0D, Tubercidin, amino acid conjugates 89-38-3D, Pteropterin, amino acid conjugates 115-02-6D, Azaserine, amino acid conjugates 127-07-1D, Hydroxyurea, amino acid conjugates 147-94-4D, Cytarabine, amino acid conjugates 148-82-3D, Melphalan, amino acid conjugates 154-42-7D, 6-Thioguanine, amino acid conjugates 154-93-8D, Carmustine, amino acid conjugates 157-03-9D, 6-Diazo-5-oxo-L-norleucine, amino acid conjugates 302-49-8D, Uredepa, amino acid conjugates 302-70-5D, Mechlorethamine oxide hydrochloride, amino acid conjugates 305-03-3D, Chlorambucil, amino acid conjugates 320-67-2D, Azacitidine, amino acid conjugates 459-86-9D, Mitoguazone, amino acid conjugates 477-30-5D, Demecolcine, amino acid conjugates 488-41-5D, Mitobronitol, amino acid conjugates 494-03-1D, Chlornaphazine, amino acid conjugates 545-55-1D, Triethylenephosphoramide, amino acid conjugates 555-77-1D, amino acid conjugates 576-68-1D, Mannomustine, amino acid conjugates 642-83-1D, Aceglatone, amino acid conjugates 645-05-6D, Altretamine, amino acid conjugates 671-16-9D, Procarbazine, amino acid conjugates 801-52-5D, Porfiromycin, amino acid conjugates 865-21-4D, Vinblastine, amino acid conjugates 1402-38-6D, Actinomycin, amino acid conjugates 1404-00-8D, Mitomycin, amino acid conjugates 1404-15-5D, Nogalamycin, amino acid conjugates 1508-45-8D, amino acid conjugates 1661-29-6D, Meturedepa, amino acid conjugates 1936-40-9D, Navembichin, amino acid conjugates 1954-28-5D, Etoglucid, amino acid conjugates 1980-45-6D, Benzodepa, amino acid conjugates 2608-24-4D, Piposulfan, amino acid conjugates 2998-57-4D, Estramustine, amino acid conjugates 3094-09-5D, Doxifluridine, amino acid conjugates 3546-10-9D, Phenesterine, amino acid conjugates 3733-81-1D, Defosfamide, amino acid conjugates 3778-73-2D, Ifosfamide, amino acid conjugates 3819-34-9D, Phenamet, amino acid conjugates 3930-19-6D, Streptonigrin, amino acid conjugates 4291-63-8D, Cladribine, amino acid conjugates 4342-03-4D, Dacarbazine, amino acid conjugates 4533-39-5D, Nitracrine, amino acid conjugates 4803-27-4D, Anthramycin, amino acid conjugates 5581-52-2D, Thiamiprine, amino acid conjugates 7440-06-4D, Platinum, complexes, amino acid conjugates 8052-16-2D, Cactinomycin, amino acid conjugates 9014-02-2D, Zinostatin, amino acid conjugates 10318-26-0D, Mitolactol, amino acid conjugates 11006-70-5D, Olivomycin, amino acid conjugates 11056-06-7D, Bleomycin, amino acid conjugates 13010-47-4D, Lomustine, amino acid conjugates 13425-98-4D, Improsulfan, amino acid conjugates 13494-90-1D, Gallium nitrate, amino acid conjugates 13665-88-8D, Mopidamol, amino acid conjugates 13909-09-6D, Semustine, amino acid conjugates

15663-27-1D, Cisplatin, amino acid conjugates 17902-23-7D, Tegafur, amino acid conjugates 18378-89-7D, Plicamycin, amino acid conjugates 18883-66-4D, Streptozocin, amino acid conjugates 20830-81-3D, Daunorubicin, amino acid conjugates 21416-67-1D, Razoxane, amino acid conjugates 21679-14-1D, Fludarabine, amino acid conjugates 22006-84-4D, Denopterin, amino acid conjugates 22089-22-1D, Trofosfamide, amino acid conjugates 23214-92-8D, Doxorubicin, amino acid conjugates 24279-91-2D, Carboquone, amino acid conjugates 24280-93-1D, Mycophenolic acid, amino acid conjugates 27778-66-1D, Tenuazonic acid, amino acid conjugates 29069-24-7D, Prednimustine, amino acid conjugates 29767-20-2D, Teniposide, amino acid conjugates 31698-14-3D, Ancitabine, amino acid conjugates 33069-62-4D, Paclitaxel, amino acid conjugates 33419-42-0D, Etoposide, amino acid conjugates 41575-94-4D, Carboplatin, amino acid conjugates 41992-23-8D, Spirogermanium, amino acid conjugates 42471-28-3D, Nimustine, amino acid conjugates 50264-69-2D, Lonidamine, amino acid conjugates 50935-04-1D, Carubicin, amino acid conjugates 51264-14-3D, Amsacrine, amino acid conjugates 52128-35-5D, Trimetrexate, amino acid conjugates 53643-48-4D, Vindesine, amino acid conjugates 53910-25-1D, Pentostatin, amino acid conjugates 54083-22-6D, Zorubicin, amino acid conjugates 54749-90-5D, Chlorozotocin, amino acid conjugates 56420-45-2D, Epirubicin, amino acid conjugates 57998-68-2D, Diaziquone, amino acid conjugates **58066-85-6D**, Miltefosine, amino acid conjugates 58337-35-2D, Elliptinium acetate, amino acid conjugates 58957-92-9D, Idarubicin, amino acid conjugates 58994-96-0D, Ranimustine, amino acid conjugates 61422-45-5D, Carmofur, amino acid conjugates 61825-94-3D, Oxaliplatin, amino acid conjugates 62435-42-1D, Perfosfamide, amino acid conjugates 65271-80-9D, Mitoxantrone, amino acid conjugates 65646-68-6D, Fenretinide, amino acid conjugates 66676-88-8D, Aclacinomycin, amino acid conjugates 68247-85-8D, Peplomycin, amino acid conjugates 70052-12-9D, Eflornithine, amino acid conjugates 71628-96-1D, Menogaril, amino acid conjugates 72496-41-4D, Pirarubicin, amino acid conjugates 72732-56-0D, Piritrexim, amino acid conjugates 74913-06-7D, Chromomycin, amino acid conjugates 78186-34-2D, Bisantrene, amino acid conjugates 80576-83-6D, Edatrexate, amino acid conjugates 85622-93-1D, Temozolomide, amino acid conjugates 92118-27-9D, Fotemustine, amino acid conjugates 95058-81-4D, Gemcitabine, amino acid conjugates 97682-44-5D, Irinotecan, amino acid conjugates 98631-95-9D, Sobuzoxane, amino acid conjugates 103775-75-3D, Miboplatin, amino acid conjugates 106486-76-4D, Carzinophilin, amino acid conjugates 110690-43-2D, Emitefur, amino acid conjugates 112887-68-0D, Tomudex, amino acid conjugates 114977-28-5D, Docetaxel, amino acid conjugates 123948-87-8D, Topotecan, amino acid conjugates
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(amino acid conjugates with drugs or with imaging agents for cancer therapy and diagnosis)

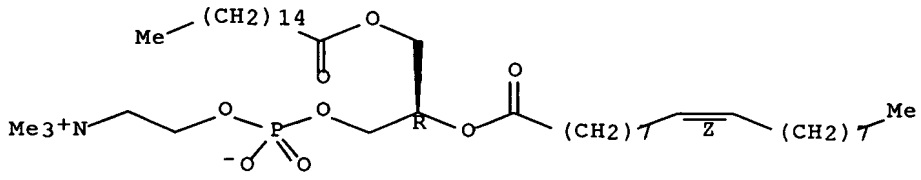
L47 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:277648 HCAPLUS Full-text
DOCUMENT NUMBER: 141:23803
TITLE: A Fourier-transform infrared spectroscopy study of sugar glasses
AUTHOR(S): Wolkers, Willem F.; Oliver, Ann E.; Tablin, Fern; Crowe, John H.
CORPORATE SOURCE: Center for Biostabilization, University of

California, Davis, CA, 95616, USA
SOURCE: Carbohydrate Research (2004), 339(6), 1077-1085
CODEN: CRBRAT; ISSN: 0008-6215
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Fourier-transform IR spectroscopy (FTIR) was used to study the hydrogen-bonding interactions that take place in vitrified carbohydrates of different chain lengths. The band position of the OH stretching band (νOH) and the shift in band position as a function of temperature were determined from the FTIR spectra as indicators for the length and strength of intermol. hydrogen bonds, resp. Differential scanning calorimetry (DSC) was used to corroborate the FTIR studies and to measure the change in heat capacity (ΔCp) that is associated with the glass transition. We found that with increasing Tg, the band position of νOH increases, the wave-number-temperature coefficient of νOH in the glassy state, WTCg, increases, whereas ΔCp decreases. The pos. correlation that was found between νOH and the glass transition temperature, Tg, indicates that the length of the hydrogen bonds increases with increasing Tg. The increase in WTCg with increasing Tg indicates that the average strength of hydrogen bonding decreases with increasing Tg. This implies that oligo- and polysaccharides (high Tg) have a greater degree of freedom to rearrange hydrogen bonds during temperature changes than monosaccharides (low Tg). Interestingly, WTCg and ΔCp showed a neg. linear correlation, indicating that the change in heat capacity during the glass transition is associated with the strength of the hydrogen-bonding network in the glassy state. Furthermore, we report that introduction of poly-L-lysine in glassy sugar matrixes decreases the average length of hydrogen bonds, irresp. of the size of the carbohydrate. Palmitoyl-oleoyl- phosphatidylcholine (POPC) vesicles were found to only interact with small sugars and not with dextran.

IT **26853-31-6**
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(interaction with small **sugars**; Fourier-transform IR spectroscopy study of **sugar** glasses)
RN 26853-31-6 HCAPLUS
CN 3,5,8-Trioxa-4-phosphahexacos-17-en-1-aminium, 4-hydroxy-N,N,N-trimethyl-9-oxo-7-[[(1-oxohexadecyl)oxy]methyl]-, inner salt, 4-oxide, (7R,17Z)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.

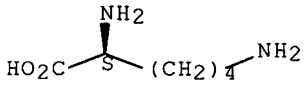


IT **25104-18-1**, L-Lysine, homopolymer
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
(poly-L-lysine introduction in glassy sugar matrixes; Fourier-transform IR spectroscopy study of sugar glasses)
RN 25104-18-1 HCAPLUS
CN L-Lysine, homopolymer (CA INDEX NAME)

CM 1

CRN 56-87-1
CMF C6 H14 N2 O2

Absolute stereochemistry.



CC 33-4 (Carbohydrates)
Section cross-reference(s): 22, 34, 75
IT **26853-31-6**
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(interaction with small **sugars**; Fourier-transform IR spectroscopy study of **sugar** glasses)
IT **25104-18-1**, L-Lysine, homopolymer
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
(poly-L-lysine introduction in glassy sugar matrixes; Fourier-transform IR spectroscopy study of sugar glasses)
REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:818459 HCAPLUS Full-text
DOCUMENT NUMBER: 139:324935
TITLE: **Polysaccharide** containing phosphorylcholine group and process for producing the same
INVENTOR(S): Miyazawa, Kazuyuki; Yanaki, Toshio; Winnik, Francoise M.
PATENT ASSIGNEE(S): Shiseido Company, Ltd., Japan
SOURCE: PCT Int. Appl., 42 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003085001	A1	20031016	WO 2003-JP4430	20030408
W: KR, US				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
JP 2003301001	A	20031021	JP 2002-106356	20020409
EP 1493754	A1	20050105	EP 2003-715780	20030408
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, SK				
US 2005222405	A1	20051006	US 2004-506771	

					200409 07
CA 2484840	A1	20060415	CA 2004-2484840		
					200410 15
PRIORITY APPLN. INFO.:			JP 2002-106356	A	
					200204 09
			WO 2003-JP4430	W	
					200304 08

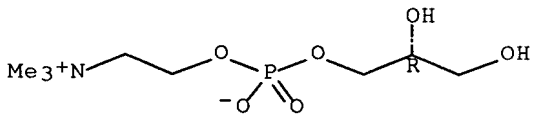
AB Disclosed are a process for producing a phosphorylcholine group-containing **polysaccharide**, characterized by causing an aldehyde-containing compound obtained by the oxidative cleavage reaction of glycerophosphorylcholine to add to an aminated **polysaccharide**; and a novel phosphorylcholine group-containing **polysaccharide** obtained by the process. The novel phosphorylcholine group-containing **polysaccharide** is excellent in biocompatibility and moisture retention and is useful as a polymeric material for medical use. This **polysaccharide** can be easily produced by the process. The **polysaccharide** is utilized in applications such as artificial organs, biomembranes, coating materials for medical supply, drug delivery, and ingredients to be incorporated in cosmetic prepns.

IT **28319-77-9DP**, L-α-Glycerophosphorylcholine, oxidative cleavage product, reaction products with aminated **polysaccharides 612845-13-3DP**, Hyaluronic acid-lysine copolymer, reaction products with oxidized glycerophosphorylcholine **612845-14-4DP**, Dextran-L-lysine copolymer, reaction products with oxidized glycerophosphorylcholine
RL: COS (Cosmetic use); IMF (Industrial manufacture); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(process for manufacture of **polysaccharide** containing phosphorylcholine group and their use in medical goods or cosmetics)

RN 28319-77-9 HCAPLUS

CN Ethanaminium, 2-[[[(2R)-2,3-dihydroxypropoxy]hydroxyphosphinyl]oxy]-N,N,N-trimethyl-, inner salt (CA INDEX NAME)

Absolute stereochemistry.



RN 612845-13-3 HCAPLUS

CN L-Lysine, polymer with hyaluronic acid (9CI) (CA INDEX NAME)

CM 1

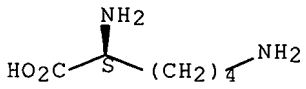
CRN 9004-61-9
CMF Unspecified
CCI PMS, MAN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

CRN 56-87-1
CMF C6 H14 N2 O2

Absolute stereochemistry.



RN 612845-14-4 HCAPLUS
CN L-Lysine, polymer with dextran (9CI) (CA INDEX NAME)

CM 1

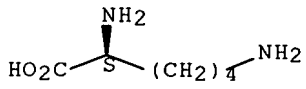
CRN 9004-54-0
CMF Unspecified
CCI PMS, MAN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

CRN 56-87-1
CMF C6 H14 N2 O2

Absolute stereochemistry.



IC ICM C08B015-00
ICS C07B037-00; C07B037-02; C07B037-08; A61K047-36; A61K007-00
CC 44-5 (Industrial Carbohydrates)
Section cross-reference(s): 62, 63
ST moisturizer medical cosmetic material coating phosphorylcholine **polysaccharide**; glycerophosphorylcholine oxidative cleavage reaction aminated **polysaccharide** addn
IT Drug delivery systems
(carriers; process for manufacture of **polysaccharide** containing phosphorylcholine group and their use in medical goods or cosmetics)
IT **Mucopolysaccharides**, preparation
Polysaccharides, preparation
RL: COS (Cosmetic use); IMF (Industrial manufacture); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(derivs.; process for manufacture of **polysaccharide** containing phosphorylcholine group and their use in medical goods or cosmetics)
IT Coating materials
(for medical goods; process for manufacture of **polysaccharide** containing phosphorylcholine group and their use in medical goods or

cosmetics)

IT Prosthetic materials and Prosthetics
(implants; process for manufacture of **polysaccharide** containing phosphorylcholine group and their use in medical goods or cosmetics)

IT Cosmetics
(moisturizers; process for manufacture of **polysaccharide** containing phosphorylcholine group and their use in medical goods or cosmetics)

IT Cosmetics
Medical goods
Membrane, biological
(process for manufacture of **polysaccharide** containing phosphorylcholine group and their use in medical goods or cosmetics)

IT 7790-28-5, Sodium periodate
RL: RGT (Reagent); RACT (Reactant or reagent)
(oxidation agent; process for manufacture of **polysaccharide** containing phosphorylcholine group and their use in medical goods or cosmetics)

IT 57-11-4DP, Stearic acid, reaction products with phosphorylcholine group-containing **polysaccharides** 143-07-7DP, Lauric acid, reaction products with phosphorylcholine group-containing **polysaccharides** 335-67-1DP, Perfluorooctanoic acid, reaction products with phosphorylcholine group-containing **polysaccharides** 9000-11-7DP, Carboxymethyl cellulose, ethylenediamine amide, reaction products with oxidized glycerophosphorylcholine, optionally esterified with fatty acids 9044-05-7DP, Carboxymethyl dextran, ethylenediamine amide, reaction products with oxidized glycerophosphorylcholine, optionally esterified with fatty acids **28319-77-9DP**, L-α-Glycerophosphorylcholine, oxidative cleavage product, reaction products with aminated **polysaccharides** **612845-13-3DP**, Hyaluronic acid-lysine copolymer, reaction products with oxidized glycerophosphorylcholine **612845-14-4DP**, Dextran-L-lysine copolymer, reaction products with oxidized glycerophosphorylcholine 612845-15-5DP, Hydroxyethyl cellulose-N-isopropylacrylamide-N-(3-aminopropyl)methacrylamide graft copolymer, reaction products with oxidized glycerophosphorylcholine
RL: COS (Cosmetic use); IMF (Industrial manufacture); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(process for manufacture of **polysaccharide** containing phosphorylcholine group and their use in medical goods or cosmetics)

IT 107-15-3DP, Ethylenediamine, reaction products with carboxymethylated **polysaccharides** 9004-61-9DP, Hyaluronic acid, ethylenediamine amide, reaction products with oxidized glycerophosphorylcholine, optionally esterified with fatty acids 9044-05-7P, Carboxymethyl dextran 53571-87-2DP, Carboxymethyl pullulan, ethylenediamine amide, reaction products with oxidized glycerophosphorylcholine, optionally esterified with fatty acids 53571-87-2P, Carboxymethyl pullulan
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(process for manufacture of **polysaccharide** containing phosphorylcholine group and their use in medical goods or cosmetics)

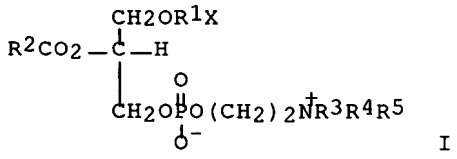
IT 79-11-8, Chloroacetic acid, reactions 9004-54-0, Dextran,

reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(process for manufacture of **polysaccharide** containing phosphorylcholine group and their use in medical goods or cosmetics)
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1989:91686 HCAPLUS Full-text
DOCUMENT NUMBER: 110:91686
TITLE: Antigenic analogs of platelet-activating factor (PAF), production of the analogs and antibodies to them, and PAF immunoassays
INVENTOR(S): Baldo, Brian Angelo; Redmond, John William
PATENT ASSIGNEE(S): University of Sydney, Australia; Macquarie University; Royal North Shore Hospital
SOURCE: PCT Int. Appl., 46 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 8705904	A1	19871008	WO 1987-AU84	19870324
W: AU, JP, KR, US RW: DE, FR, GB, IT				
AU 8772097	A	19871020	AU 1987-72097	19870324
AU 607698	B2	19910314		
EP 299965	A1	19890125	EP 1987-902318	19870324
R: DE, FR, GB, IT				
JP 01502584	T	19890907	JP 1987-502157	19870324
IL 82057	A	19941111	IL 1987-82057	19870331
US 5061626	A	19911029	US 1987-156923	19871124
PRIORITY APPLN. INFO.:			AU 1986-5175 A	19860324
			WO 1987-AU84 A	19870324

OTHER SOURCE(S): MARPAT 110:91686
GI



I

AB PAF analogs I [R1 = C2-25 alkylene or alkenylene linking group substituted by radioactive I and X = H; or R1 = C2-25 alkylene, alkenylene, alkynylene, optionally 3H- or radioactive I-substituted, and X = CHO, di(C1-6 alkoxy)methyl, CO2H, NCO, OH, SH, N-(C1-6 alkyl)amino, N,N-di(C1-6 alkyl)amino, AB; A = linking group (NR6, CO2, O2C, CONR6, NR6CO, NHCSNH, SS; R6 = H, C1-6 alkyl); B = protein, peptide, carbohydrate, lipid of ≥2000 mol. weight, label; R2-R5 = C1-6 alkyl] are prepared and are useful in production of anti-PAF antibodies or as reagents in PAF immunoassays. 2-O-Acetyl-1-O-(6'-oxohexyl)-sn-glyceryl-3-phosphorylcholine [prepared from cyclohexanone and HC(OMe)3 in 8 steps] was conjugated to methylated bovine serum albumin. The conjugate was used to prepare rabbit anti-PAF serum which was used in an assay for PAF.

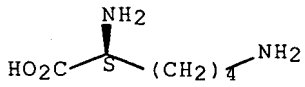
IT **25104-18-1D**, Polylysine, glycerylphosphorylcholine derivative conjugates **119142-22-2D**, albumin and polylysine conjugates
RL: ANST (Analytical study)
(as antigenic blood platelet-activating factor analogs)

RN 25104-18-1 HCAPLUS
CN L-Lysine, homopolymer (CA INDEX NAME)

CM 1

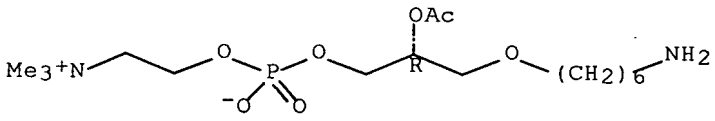
CRN 56-87-1
CMF C6 H14 N2 O2

Absolute stereochemistry.



RN 119142-22-2 HCAPLUS
CN 3,5,9-Trioxa-4-phosphapentadecan-1-aminium, 7-(acetyloxy)-15-amino-4-hydroxy-N,N,N-trimethyl-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

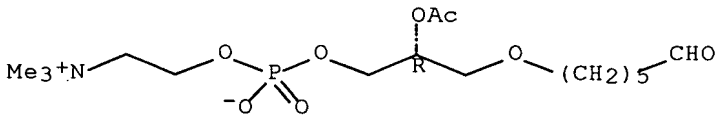
Absolute stereochemistry.



IT **119142-21-1DP**, methylated albumin conjugates
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as immunogen for blood platelet-activating factor

immunoassay)
RN 119142-21-1 HCAPLUS
CN 3,5,9-Trioxa-4-phosphapentadecan-1-aminium, 7-(acetyloxy)-4-hydroxy-N,N,N-trimethyl-15-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07F009-10
ICS G01N033-92; C07K015-12
CC 9-10 (Biochemical Methods)
Section cross-reference(s): 7, 23, 29
IT Carbohydrates and **Sugars**, compounds
RL: ANST (Analytical study)
(acetals, in blood platelet-activating factor determination in body fluid by immunoassay)
IT Carbohydrates and **Sugars**, esters
RL: ANST (Analytical study)
(alditols, anhydro, esters, with fatty acids, alkyl ethers, in blood platelet-activating factor determination in body fluid by immunoassay)
IT Albumins, compounds
Carbohydrates and **Sugars**, compounds
Lipids, compounds
Peptides, compounds
Proteins, specific or class
RL: ANST (Analytical study)
(conjugates, with glycerylphosphorylcholine derivative, as antigenic blood platelet-activating factor analogs)
IT Carbohydrates and **Sugars**, esters
RL: ANST (Analytical study)
(hexitols, anhydro, esters, with fatty acids, alkyl ethers, in blood platelet-activating factor determination in body fluid by immunoassay)
IT **25104-18-1D**, Polylysine, glycerylphosphorylcholine derivative conjugates 38000-06-5D, Polylysine, glycerylphosphorylcholine derivative conjugates **119142-22-2D**, albumin and polylysine conjugates
RL: ANST (Analytical study)
(as antigenic blood platelet-activating factor analogs)
IT **119142-21-1DP**, methylated albumin conjugates
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as immunogen for blood platelet-activating factor immunoassay)

=> d l49 ibib abs hitstr hitind 1-34

L49 ANSWER 1 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:353984 HCAPLUS Full-text
DOCUMENT NUMBER: 141:167347
TITLE: S-1-O-phosphocholine-2-N-acetyloctadecane induces apoptosis in T cells: involvement of

receptor activation and the intrinsic apoptotic pathway

AUTHOR(S): Oberle, Carolin; Massing, Ulrich; Krug, Harald F.

CORPORATE SOURCE: Forschungszentrum Karlsruhe, Institute of Toxicology and Genetics, Karlsruhe, Germany

SOURCE: Signal Transduction (**2003**), Volume Date 2004, 3(5-6), 218-231
CODEN: STIRCI; ISSN: 1615-4053

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

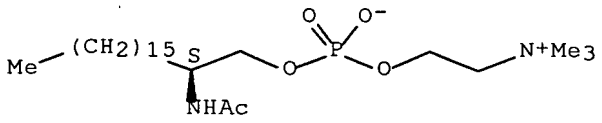
AB Alkylphosphocholines (APC) represent compds. with far-ranging biol. activities including inhibition of neoplastic cell growth in vivo and in vitro. Here we introduce the apoptosis-inducing activity of a newly synthesized APC, the S-NC-2, in Jurkat T cells. The results point to a dual apoptotic mechanism, a death receptor dependent activation as well as a death receptor-independent and mitochondria related pathway. The participation of the CD95 death receptor was determined by immunohistochem. Receptor aggregation and capping was already induced after 2 h of treatment with S-NC-2. We further analyzed phosphatidylserine externalization, chromatin condensation, the cleavage of procaspases-8, -9 and -3 and the degradation of caspase substrates. Comparison of Jurkat wildtype with FADD- and caspase-8-deficient cells and, addnl., the Bcl-2 overexpressing variant revealed a more detailed model of the APC-induced apoptosis. The lack of FADD or caspase-8 resulted in a somehow decreased amount of apoptotic cells, whereas the overexpression of Bcl-2 leads to a complete reduction of apoptosis and caspase-activation. After stimulation of death receptors such as CD95, the amplification via intrinsic apoptotic pathways is strongly required in Type II T cells.

IT **156991-58-1**
RL: PAC (Pharmacological activity); BIOL (Biological study)
(S-1-O-phosphocholine-2-N-acetyloctadecane induces apoptosis in T cells: involvement of receptor activation and the intrinsic apoptotic pathway)

RN 156991-58-1 HCAPLUS

CN 3,5-Dioxa-8-aza-4-phosphadecan-1-aminium, 7-hexadecyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (7S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 1-6 (Pharmacology)

IT **156991-58-1**
RL: PAC (Pharmacological activity); BIOL (Biological study)
(S-1-O-phosphocholine-2-N-acetyloctadecane induces apoptosis in T cells: involvement of receptor activation and the intrinsic apoptotic pathway)

REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 2 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:657127 HCAPLUS Full-text

DOCUMENT NUMBER: 139:347335
TITLE: Solution Properties of Hydrophobically Modified Phosphorylcholine-Based Polymers in Water and in the Presence of Surfactants
AUTHOR(S): Miyazawa, Kazuyuki; Winnik, Francoise M.
CORPORATE SOURCE: Department of Chemistry and Faculty of Pharmacy, Universite de Montreal, Montreal, QC, H3C 3J7, Can.
SOURCE: Journal of Physical Chemistry B (**2003**), 107(38), 10677-10682
CODEN: JPCBFK; ISSN: 1520-6106
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The photophys. properties of a fluorescently labeled amphiphilic polybetaine have been investigated by steady state and time-resolved fluorescence spectroscopy. The copolymer consists of N-isopropylacrylamide and N-phosphorylcholine-N'-ethylenedioxybis(ethyl)acrylamide units in .apprx.1/1 molar ratio, as well as 5 mol % of N-[(1-pyrenyl)-4-butyl]-N-n- (octadecyl)acrylamide. In water, individual copolymer chains associate in multichain aggregates held together by hydrophobic interactions between the hydrocarbon chains and by ion pair formation between the phosphorylcholine groups. By monitoring the changes in the ratio of the pyrene excimer emission intensity (IE) to the pyrene monomer emission intensity (IM), we established (1) that the polymer assemblies are disrupted by the addition of divalent salts, such as CaCl2 and (2) that interactions take place between the polymer and anionic, cationic, zwitterionic, or neutral surfactants. The mechanism of binding is discussed in terms of surfactant charge and chain length and compared to the association of surfactant to a copolymer of N-isopropylacrylamide and N-phosphorylcholine-N'- ethylenedioxybis(ethyl)acrylamide devoid of hydrophobic substituents.

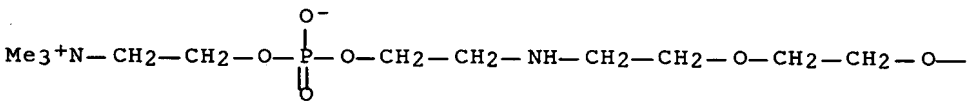
IT **547744-01-4**, PNIPAM-PC **618912-21-3**, PNIPAM-PC-c18Py
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
(solution properties of hydrophobically modified phosphorylcholine-based polymers in water are affected by electrolytes and surfactants)

RN 547744-01-4 HCAPLUS
CN 3,5,11,14-Tetraoxa-8,17-diaza-4-phosphaeicos-19-en-1-aminium, 4-hydroxy-N,N,N-trimethyl-18-oxo-, inner salt, 4-oxide, polymer with N-(1-methylethyl)-2-propenamide (9CI) (CA INDEX NAME)

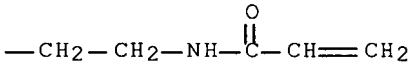
CM 1

CRN 547744-00-3
CMF C16 H34 N3 O7 P

PAGE 1-A

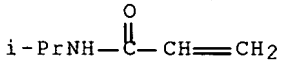


PAGE 1-B



CM 2

CRN 2210-25-5
CMF C6 H11 N O

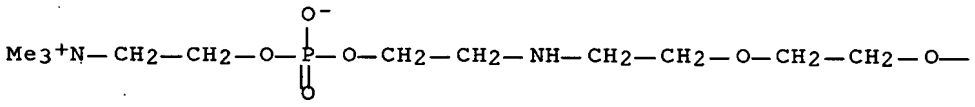


RN 618912-21-3 HCAPLUS
CN 3,5,11,14-Tetraoxa-8,17-diaza-4-phosphaeicos-19-en-1-aminium, 4-hydroxy-N,N,N-trimethyl-18-oxo-, inner salt, 4-oxide, polymer with N-(1-methylethyl)-2-propenamide and N-octadecyl-N-[4-(1-pyrenyl)butyl]-2-propenamide (9CI) (CA INDEX NAME)

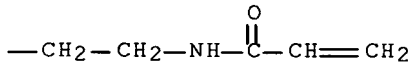
CM 1

CRN 547744-00-3
CMF C16 H34 N3 O7 P

PAGE 1-A

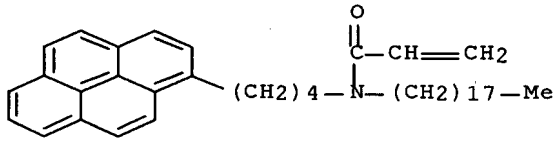


PAGE 1-B



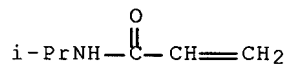
CM 2

CRN 129674-15-3
CMF C41 H57 N O



CM 3

CRN 2210-25-5
CMF C6 H11 N O



CC 6-7 (General Biochemistry)
IT **547744-01-4**, PNIPAM-PC **618912-21-3**,
PNIPAM-PC-c18Py
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
(solution properties of hydrophobically modified phosphorylcholine-based polymers in water are affected by electrolytes and surfactants)
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 3 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:291718 HCAPLUS Full-text
DOCUMENT NUMBER: 139:54595
TITLE: Isothermal titration calorimetry and fluorescence spectroscopy studies of the interactions between surfactants and a phosphorylcholine-based polybetaine
AUTHOR(S): Miyazawa, Kazuyuki; Winnik, Francoise M.
CORPORATE SOURCE: Department of Chemistry and Faculty of Pharmacy, Universite de Montreal, CP 6128 Succursale Centre Ville, Montreal, QC, H3C 3J7, Can.
SOURCE: Progress in Colloid & Polymer Science (**2003**), 122, 149-156
CODEN: PCPSD7; ISSN: 0340-255X
PUBLISHER: Springer
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The interactions between a polybetaine and anionic, cationic, zwitterionic and neutral surfactants were studied by a fluorescence experiment with pyrene as a probe, isothermal titration calorimetry, and 1H NMR spectroscopy. The polybetaine was a phosphorylcholine-based polymer (PNIPAM-PC) consisting of equimolar amts. of N-isopropylacrylamide and N-phosphorylcholine-N'-ethylenedioxybis(ethyl)acrylamide. Strong association took place between PNIPAM-PC and the anionic surfactants sodium n-dodecyl sulfate (SDS) and sodium n-hexadecyl sulfate (SHS) via a cooperative mechanism driven by electrostatic interactions between the surfactant headgroup and the trimethylammonium group of the PC (phosphorylcholine) moiety linked to the polymer. The onset of binding between PNIPAM-PC and SDS or SHS takes place for surfactant concns. of 2.0 and 0.028 mmol l-1, resp., which are lower than their resp. critical micelle concns. (8.3 and 0.058 mmol·l-1). No interactions were detected between PNIPAM-PC and zwitterionic surfactants bearing either a phosphorylcholine headgroup (n-hexadecanoyl lysophosphocholine) or a dimethyl-3-ammonio-1- propanesulfonate group, cationic surfactants bearing a trimethylammonium headgroup, or neutral surfactants bearing a hepta(ethyleneglycol) headgroup. The mechanism of binding

is discussed in terms of surfactant charge and chain length and is compared to the association of surfactants to polyampholytes and polyelectrolytes.

IT **547744-01-4**
RL: PRP (Properties)
(isothermal titration calorimetry and fluorescence spectroscopy studies of interactions between surfactants and phosphorylcholine-based polybetaine)

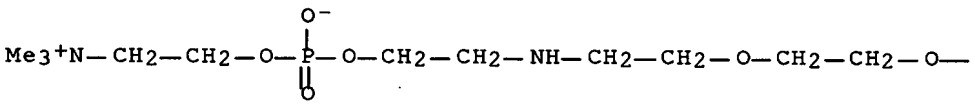
RN 547744-01-4 HCAPLUS

CN 3,5,11,14-Tetraoxa-8,17-diaza-4-phosphaeicos-19-en-1-aminium, 4-hydroxy-N,N,N-trimethyl-18-oxo-, inner salt, 4-oxide, polymer with N-(1-methylethyl)-2-propenamide (9CI) (CA INDEX NAME)

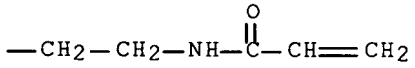
CM 1

CRN 547744-00-3
CMF C16 H34 N3 O7 P

PAGE 1-A



PAGE 1-B



CM 2

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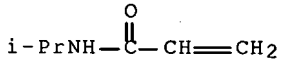


CC 46-3 (Surface Active Agents and Detergents)
Section cross-reference(s): 37

IT 112-02-7 151-21-3, Sodium dodecyl sulfate, properties 1119-94-4, N-Dodecyl-N,N,N-trimethylammonium bromide 1120-01-0, Sodium n-hexadecyl sulfate 2281-11-0, N-Hexadecyl-N,N-dimethyl-3-ammonio-1-propanesulfonate 14933-08-5, N-Dodecyl-N,N-dimethyl-3-ammonio-1-propanesulfonate 17364-16-8 **547744-01-4**
RL: PRP (Properties)
(isothermal titration calorimetry and fluorescence spectroscopy studies of interactions between surfactants and phosphorylcholine-based polybetaine)

REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 4 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:112917 HCAPLUS Full-text
DOCUMENT NUMBER: 138:158547
TITLE: Phosphorylcholine group-containing polymers, their manufacture, and topical preparations
INVENTOR(S): Miyazawa, Kazuyuki; Hariki, Toshio; Winnik, Francoise
PATENT ASSIGNEE(S): Shiseido Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003040942	A	20030213	JP 2002-61759	20020307
			<--	
PRIORITY APPLN. INFO.:			JP 2001-152309	A 20010522
			<--	

AB Polymers having phosphorylcholine groups are manufactured by reaction of polymers containing amino groups with compds. containing aldehydes prepared by oxidative cleavage of glycerophosphorylcholine. Octadecylacrylamide-N-isopropylacrylamide-N-[2-[2-(2- aminoethoxy)ethoxy]ethyl]methacrylamide copolymer (preparation given) was treated with an aldehyde prepared by oxidative cleavage of L-α-glycerophosphorylcholine and the product was reduced with NaBH3CN to give a phosphorylcholine group-containing polymer. A topical preparation containing sorbitol 8, 1,3-butylene glycol 5, EtOH 7, polyoxyethylene oleyl ether 1, olive oil 0.2, the phosphorylcholine group-containing polymer 0.1, and H2O to 100 weight% showed skin-moisturizing and -softening effects. The polymer enhanced percutaneous absorption of arbutin.

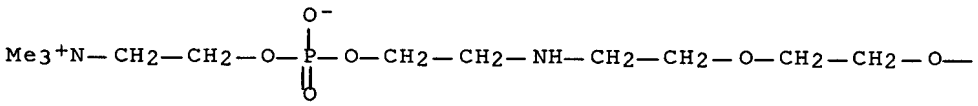
IT **496801-31-1P**
RL: BSU (Biological study, unclassified); COS (Cosmetic use); IMF (Industrial manufacture); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(manufacture of phosphorylcholine group-containing polymers for topical prepns.)

RN 496801-31-1 HCAPLUS
CN 3,5,11,14-Tetraoxa-8,17-diaza-4-phosphaeicos-19-en-1-aminium, 4-hydroxy-N,N,N,19-tetramethyl-18-oxo-, inner salt, 4-oxide, polymer with N-(1-methylethyl)-2-propenamide and N-octadecyl-2-propenamide (9CI) (CA INDEX NAME)

CM 1

CRN 496801-24-2
CMF C17 H36 N3 O7 P

PAGE 1-A



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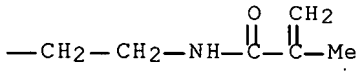
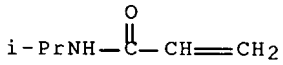


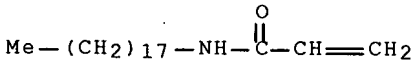
CM 2

CRN 2210-25-5
CMF C6 H11 N O



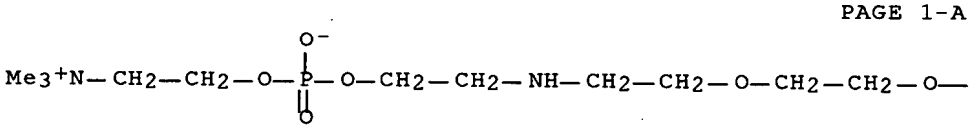
CM 3

CRN 1506-54-3
CMF C21 H41 N O



IT **496801-24-2P**
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(manufacture of phosphorylcholine group-containing polymers for topical prepns.)
RN 496801-24-2 HCAPLUS
CN 3,5,11,14-Tetraoxa-8,17-diaza-4-phosphaeicos-19-en-1-aminium, 4-hydroxy-N,N,N,19-tetramethyl-18-oxo-, inner salt, 4-oxide (9CI) (CA INDEX NAME)

PAGE 1-A



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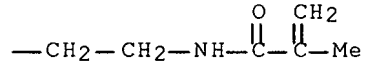


IC ICM C08F230-02
ICS A61K007-00; A61K007-48; A61K031-80; A61P017-16
CC 62-4 (Essential Oils and Cosmetics)
Section cross-reference(s): 35, 37, 63
IT 25104-18-1DP, Polylysine, reaction products with glycerophosphorylcholine oxidative cleavage product 28319-77-9DP, L-α-Glycerophosphorylcholine, oxidative cleavage product, reaction products with amino-containing polymers 30551-89-4DP, Polyallylamine, reaction products with glycerophosphorylcholine oxidative cleavage product 38000-06-5DP, Polylysine, reaction products with glycerophosphorylcholine oxidative cleavage product 496800-94-3DP, reaction products with glycerophosphorylcholine oxidative cleavage product 496800-97-6DP, reaction products with glycerophosphorylcholine oxidative cleavage product 496801-03-7DP, reaction products with glycerophosphorylcholine oxidative cleavage product 496801-11-7DP, reaction products with glycerophosphorylcholine oxidative cleavage product 496801-25-3P **496801-31-1P**
RL: BSU (Biological study, unclassified); COS (Cosmetic use); IMF (Industrial manufacture); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(manufacture of phosphorylcholine group-containing polymers for topical prepns.)
IT 496801-15-1P **496801-24-2P**
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(manufacture of phosphorylcholine group-containing polymers for topical prepns.)

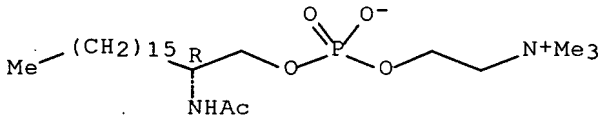
L49 ANSWER 5 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:148901 HCAPLUS Full-text
DOCUMENT NUMBER: 135:162145
TITLE: Killing tumour cells by alkylphosphocholines: Evidence for involvement of CD95
AUTHOR(S): Matzke, Astrid; Massing, Ulrich; Krug, Harald F.
CORPORATE SOURCE: Forschungszentrum Karlsruhe, Institute for Toxicology and Genetics, Karlsruhe, D-76021, Germany
SOURCE: European Journal of Cell Biology (**2001**), 80(1), 1-10
CODEN: EJCBDN; ISSN: 0171-9335
PUBLISHER: Urban & Fischer Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Many lipids act as cellular messengers and lead to a variety of different cellular responses. Out of the group of these compds. the ceramides are able to induce apoptosis, and some synthetic lipids can mimic this effect. Apoptosis is an important mechanism whereby chemotherapeutics exhibit their anti-oncogenic activity. Although, some lipid analogs were used in clin. trials, they exert severe side effects and their mechanism of action is widely unknown. The authors present here a new class of synthetic alkylphosphocholines (APC) that induce programmed cell death in leukemia cells. The signs of apoptosis arise after 1 h of incubation with these compds. as shown by phosphatidylserine externalization

followed by caspase activation and DNA fragmentation. The authors demonstrate that the mol. target of these lipids is upstream of caspases and Bcl-2. Expts. with FADD dominant neg. cells reveal that induction of apoptosis occurs on the level of CD95 and that these compds. can now be optimized for their capacity to activate the apoptosis-inducing receptor CD95.

IT **156991-49-0 156991-58-1**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(apoptosis induction by alkylphosphocholines)

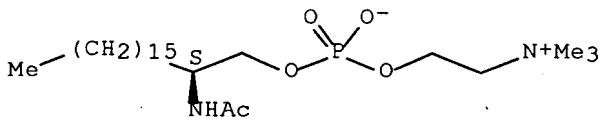
RN 156991-49-0 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphadecan-1-aminium, 7-hexadecyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 156991-58-1 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphadecan-1-aminium, 7-hexadecyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (7S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 1-6 (Pharmacology)

IT 156991-44-5 **156991-49-0** 156991-53-6 **156991-58-1**
157478-43-8 157478-44-9 157478-49-4 157478-50-7
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(apoptosis induction by alkylphosphocholines)

REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 6 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:452505 HCAPLUS Full-text
DOCUMENT NUMBER: 133:79408
TITLE: Ammonium phosphate-containing polymers, lenses using them, and their manufacture
INVENTOR(S): Sato, Toshihiro; Kurosaki, Juichi
PATENT ASSIGNEE(S): Nippon Contact Lens KK, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 17 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent

LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000186117	A	20000704	JP 1998-365486 <--	199812 22
PRIORITY APPLN. INFO.:			JP 1998-365486 <--	199812 22

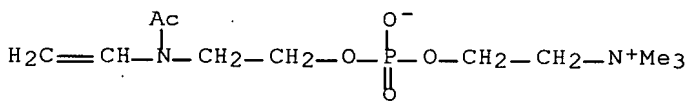
AB The polymers are manufactured using CH2:CHNXY [X = COR1, R1; R1 = H, (halo)alkyl, (halo)aryl; Y = AOP(O)(O-)OBN+R2R3R4, ER5R6N+DOP(O)(O-)OR7; A = C1-20 alkylene, (CH2CH2O)nCH2CH2, (CH2CHMeO)nCH2CMeH ; n = 1-8; B, D = (CH2)m, CH2CMeH, CH2CMe2CH2; m = 1-3; R2-R6 = (hydroxy)alkyl, aryl; E = C1-8 alkylene; R5 - R6 = (hydroxy)alkyl, aryl; R7 = (halo)alkyl, (halo)aryl, R8NR9R10; R8 = alkylene, phenylene; R9, R10 = H, alkyl]. A contact lens comprising 40/55/4/1 2-(N-ethyl-N-vinyl)aminoethyl 2'-(trimethylammonio)ethyl phosphate-2-hydroxyethyl methacrylate-Me methacrylate-vinyl methacrylate copolymer showed water content 68.2%, strength and elongation at break 11 kg/cm2 and 215%, resp., and good resistance to protein deposition.

IT **279687-32-0P 279687-39-7P**, 2-(N-Acetyl-N-vinyl)aminoethyl-2'-(trimethylammonio)ethyl phosphate-allyl methacrylate-2-hydroxyethyl methacrylate-N,N'-methylenebismethacrylamide-2,2,2-trifluoro-1-trifluoromethylethyl methacrylate copolymer **279687-44-4P**, 2-(N-Acetyl-N-vinyl)aminoethyl 2'-(trimethylammonio)ethyl phosphate-methacryloxyethoxypropyltris(trimethylsiloxy)silane-N,N'-methylenebismethacrylamide-methyl methacrylate-triethylene glycol dimethacrylate-2,2,2-trifluoro-1-(trifluoromethyl)ethyl methacrylate copolymer
RL: DEV (Device component use); IMF (Industrial manufacture); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(resistance to soiling; ammonium phosphate-containing polymers for contact lens with excellent moisture retension and stain prevention and removal)

RN 279687-32-0 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphadec-9-en-1-aminium, 8-acetyl-4-hydroxy-N,N,N-trimethyl-, inner salt, 4-oxide, polymer with 2-hydroxyethyl 2-methyl-2-propenoate, N,N'-methylenebis[2-propenamide] and methyl 2-methyl-2-propenoate (9CI) (CA INDEX NAME)

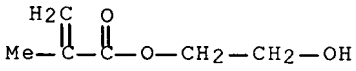
CM 1

CRN 279687-31-9
CMF C11 H23 N2 O5 P



CM 2

CRN 868-77-9
CMF C6 H10 O3



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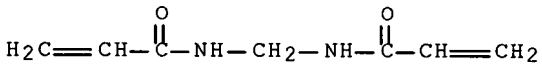
CRN 110-26-9
CMF C7 H10 N2 O2



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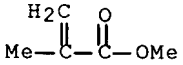
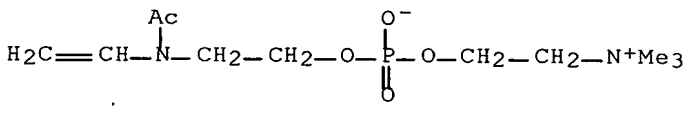


RN 279687-39-7 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphadec-9-en-1-aminium, 8-acetyl-4-hydroxy-N,N,N-trimethyl-, inner salt, 4-oxide, polymer with 2-hydroxyethyl 2-methyl-2-propenoate, N,N'-methylenebis[2-methyl-2-propenamide], 2-propenyl 2-methyl-2-propenoate and 2,2,2-trifluoro-1-(trifluoromethyl)ethyl 2-methyl-2-propenoate (9CI) (CA INDEX NAME)

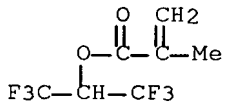
CM 1

CRN 279687-31-9
CMF C11 H23 N2 O5 P



CM 2

CRN 3063-94-3
CMF C7 H6 F6 O2



CM 3

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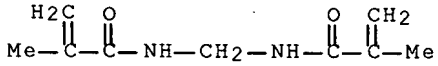
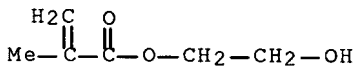


CM 4

CRN 868-77-9
CMF C6 H10 O3



CM 5

CRN 96-05-9
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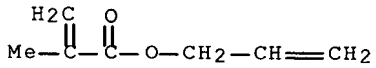
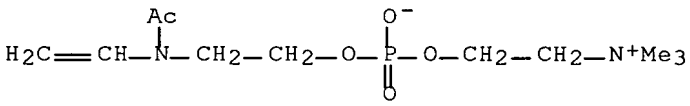


RN 279687-44-4 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphadec-9-en-1-aminium, 8-acetyl-4-hydroxy-N,N,N-trimethyl-, inner salt, 4-oxide, polymer with 1,2-ethanediylbis(oxy-2,1-ethanediyl) bis(2-methyl-2-propenoate), N,N'-methylenebis[2-methyl-2-propenamide], methyl 2-methyl-2-propenoate, 2,2,2-trifluoro-1-(trifluoromethyl)ethyl 2-methyl-2-propenoate and 2-[3-[3,3,3-trimethyl-1,1-bis[(trimethylsilyl)oxy]disiloxanyl]propoxy]ethyl 2-methyl-2-propenoate (9CI) (CA INDEX NAME)

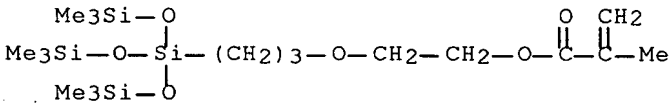
CM 1

CRN 279687-31-9
CMF C11 H23 N2 O5 P



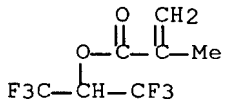
CM 2

CRN 104512-64-3
CMF C18 H42 O6 Si4



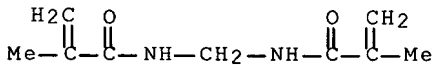
CM 3

CRN 3063-94-3
CMF C7 H6 F6 O2



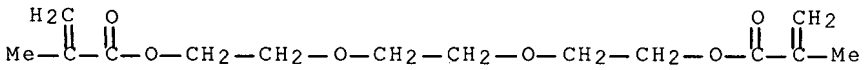
CM 4

CRN 2359-15-1
CMF C9 H14 N2 O2



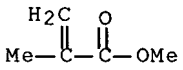
CM 5

CRN 109-16-0
CMF C14 H22 O6



CM 6

CRN 80-62-6
CMF C5 H8 O2



IC ICM C08F030-00
ICS G02B001-04
CC 63-7 (Pharmaceuticals)
Section cross-reference(s): 38
IT 279687-30-8P, 2-(N-Ethyl-N-vinyl)aminoethyl-2'-(trimethylammonio)ethyl phosphate-2-hydroxyethyl methacrylate-methyl methacrylate-vinyl methacrylate copolymer **279687-32-0P** 279687-34-2P 279687-36-4P, N,N-Dimethylacrylamide-5-(N-ethyl-N-vinyl)aminoethoxyethyl 2'-(triethylammonio)ethyl phosphate-N,N'-methylenebisacrylamide-methyl methacrylate copolymer 279687-37-5P, 3-(N-Acetyl-N-vinyl)aminopropyl 2'-(triethanolammonio)ethyl phosphate-allyl methacrylate-methyl methacrylate-vinyl methacrylate-N-vinyl-2-pyrrolidone copolymer **279687-39-7P**, 2-(N-Acetyl-N-vinyl)aminoethyl-2'-(trimethylammonio)ethyl phosphate-allyl methacrylate-2-hydroxyethyl methacrylate-N,N'-methylenebismethacrylamide-2,2,2-trifluoro-1-trifluoromethylethyl methacrylate copolymer 279687-41-1P 279687-43-3P, 2-[[2-(N-Acetyl-N-vinylaminoethyl]dimethylammonium]ethyl hexafluoroisopropyl phosphate-N,N-dimethylacrylamide-N,N'-methylenebismethacrylamide-methyl methacrylate-vinyl methacrylate copolymer **279687-44-4P**, 2-(N-Acetyl-N-vinyl)aminoethyl 2'-(trimethylammonio)ethyl phosphate-methacryloxyethoxypropyltris(trimethylsiloxy)silane-N,N'-methylenebismethacrylamide-methyl methacrylate-triethylene glycol dimethacrylate-2,2,2-trifluoro-1-(trifluoromethyl)ethyl methacrylate copolymer 279687-45-5P, 3-(N-Acetyl-N-vinyl)aminopropyl 2'-(triethanolammonio)ethyl phosphate-methacryloxyethoxypropyltris(trimethylsiloxy)silane-N,N'-methylenebismethacrylamide-methyl methacrylate-triethylene glycol, dimethacrylate-2,2,2-trifluoro-1-(trifluoromethyl)ethyl methacrylate copolymer 279687-47-7P, 5-(N-Acetyl-N-vinyl)aminoethoxyethyl 2'-(trimethylammonio)ethyl phosphate-ethylene glycol dimethacrylate-methacryloxyethoxypropyltris(trimethylsiloxy)silane-N,N'-methylenebismethacrylamide-methyl methacrylate-2,2,2-trifluoroethyl methacrylate copolymer 279687-48-8P, 2-[[2-(N-Acetyl-N-vinyl)aminoethyl]dimethylammonium]ethyl hexafluoroisopropyl phosphate-allyl methacrylate-methacrylic acid-methacryloxyethoxypropyltris(trimethylsiloxy)silane-methyl methacrylate-triethylene glycol, dimethacrylate-2,2,2-trifluoro-1-(trifluoromethyl)ethyl methacrylate copolymer
RL: DEV (Device component use); IMF (Industrial manufacture); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(resistance to soiling; ammonium phosphate-containing polymers for

contact lens with excellent moisture retension and stain prevention and removal)

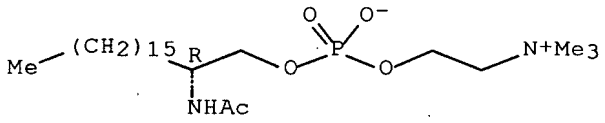
L49 ANSWER 7 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:180745 HCAPLUS Full-text
DOCUMENT NUMBER: 132:342804
TITLE: Alkylphosphocholines - a new class of antitumor agents: studies of their biochemical action mechanism
AUTHOR(S): Matzke, Astrid
CORPORATE SOURCE: Inst. Toxikologie Genetik, Germany
SOURCE: Wissenschaftliche Berichte - Forschungszentrum Karlsruhe (**1999**), FZKA 6369, a-b, i-v, 1-106
CODEN: WBFKF5; ISSN: 0947-8620
DOCUMENT TYPE: Report
LANGUAGE: German

AB Alkylphosphocholines (APC) represent a new class of anticancer drugs. Although some compds. of this group are already used for tumor therapy (e.g. hexadecylphosphocholine, HePC), not much is known about their mol. mechanisms of anticancerogenic action. HePC is approved for topical treatment of skin metastases of breast cancer, but systemic application is not possible due to gastrointestinal side effects. Therefore, new APC compds. were synthesized with the aim to reduce the side effects of HePC while preserving the antineoplastic activities. In the present study, the toxic effects of 8 new APC compds. on in vitro cell culture systems of human tumor cells were investigated. 3 Of the new APC showed higher toxic potency than HePC towards HL-60 leukemia cells. The most active compound was R-1-O-phosphocholine-2-N-acetyl-octadecane (R-N-acetyl), with which further studies were mainly carried out. The uptake of R-N-acetyl by tumor cells was slow and dependent on the content of fetal calf serum in the culture media. R-N-acetyl was metabolically stable and degradation was only marginal. The effect of APC on intracellular signal transduction was further specified. It was demonstrated that APC activate the Ras/MAP kinase cascade via a G-protein coupled mechanism. The EGF-receptor was engaged in the activation of the MAP kinase ERK in MDA-MB-468 mammary carcinoma cells. Furthermore, APC induced concentration-dependent a short, transient, and receptor-mediated rise in cytosolic free Ca. In the 2nd part of the thesis, the APC-induced programmed cell death was investigated. Deregulation of apoptosis is characteristic for tumor cells. Agents which compensate for this defect and which are able to selectively induce apoptotic cell death of tumor cells are of great interest for tumor therapy. Using different microscopical and biochem. techniques, cell death was identified unequivocally as apoptosis. After treatment with APC, apoptosis was induced within several hours and was not dependent on the cell system investigated. The activation of caspases and endonucleases is responsible for the highly specific degradation processes observed after treatment with APC. This was demonstrated by pretreatment with specific caspase inhibitors which led to an inhibition of APC-induced effects and to the rescue from apoptotic cell death. Furthermore, overexpression of the anti- apoptotic protein bcl-2 was a protection from APC induced cell death dependent on the cell system. The death receptor CD95 (Fas/APO-1) could be identified as a regulatory element in APC- induced apoptosis, which represents a possible target for APC at the plasma membrane. The new alkylphosphocholine compds. can now be optimized for their capacities to activate CD95 and for the application for tumor therapy.

IT **156991-49-0 156991-58-1**
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(alkylphosphocholines, studies of their biochem. action mechanism)

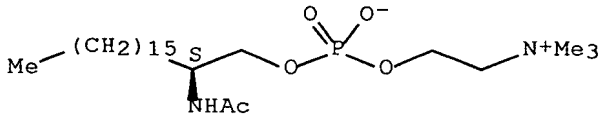
RN 156991-49-0 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphadecan-1-aminium, 7-hexadecyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 156991-58-1 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphadecan-1-aminium, 7-hexadecyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (7S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 1-3 (Pharmacology)
IT 156991-44-5 **156991-49-0** 156991-53-6 **156991-58-1**
157478-43-8 157478-44-9 157478-49-4 157478-50-7
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(alkylphosphocholines, studies of their biochem. action mechanism)
REFERENCE COUNT: 162 THERE ARE 162 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 8 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:573628 HCAPLUS Full-text
DOCUMENT NUMBER: 131:333906
TITLE: Enzymatic properties of rat group IIA and V phospholipases A2 compared
AUTHOR(S): Janssen, M. J. W.; Vermeulen, L.; Van der Helm, H. A.; Aarsman, A. J.; Slotboom, A. J.; Egmond, M. R.
CORPORATE SOURCE: Faculty of Chemistry, Centre for Biomembranes and Lipid Enzymology (Institute of Biomembranes), Department of Enzymology and Protein Engineering, Utrecht University, Utrecht, 3508 TB, Neth.
SOURCE: Biochimica et Biophysica Acta, Molecular and Cell Biology of Lipids (**1999**), 1440(1), 59-72
CODEN: BBMLFG; ISSN: 1388-1981
PUBLISHER: Elsevier B.V.

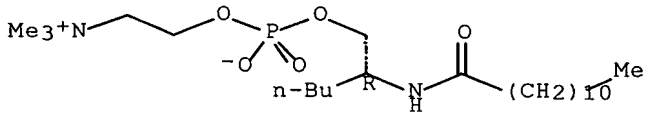
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Group IIA and V phospholipases A2 (PLA2s) are known to play a role in inflammatory responses. We have constructed a bacterial expression vector for rat group IIA and V PLA2s, over-expressed, folded and purified the proteins with the aim to study and compare the properties of the enzymes in detail. For zwitterionic phospholipid micelles, both enzymes display optimum activity at pH 8.0 and absolutely require Ca2+ for enzymic activity. In the presence of substrate, group V PLA2 has a high affinity for Ca2+ (KCa2+=90 μM) while KCa2+ of group IIA PLA2 was found to be 1.6 mM. The absence of substrate only marginally influences the Ca2+ affinities. In contrast to group IIA PLA2, group V PLA2 does not show a jump in the activity profile at substrate concns. around the critical micelle concentration Direct binding studies using n-alkylphosphocholines indicate that group V PLA2 forms protein-lipid aggregates at pre-micellar lipid concns. in a cooperative and Ca2+-dependent manner. This behavior, which is comparable to that observed for the PLA2 from Naja melanoleuca snake venom, reflects the high affinity of this enzyme for zwitterionic phospholipids. Competitive inhibition by the substrate analogs (R)-2-dodecanoylaminohexanol-1-phosphocholine and its phosphoglycol derivative was tested on zwitterionic micelles as substrate. Group IIA PLA2 shows a preference for the phosphoglycol inhibitor whereas the phosphocholine inhibitor binds stronger to the active site of group V PLA2. The enzymic activity was also measured on zwitterionic liposomes which appear to be much better substrates for group V PLA2 than for group IIA PLA2. The overall results suggest that group V PLA2 is better suited for action on biol. membranes than group IIA PLA2.

IT **131736-68-0**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(enzymic properties of rat group IIA and V phospholipases A2 compared)

RN 131736-68-0 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 7-3 (Enzymes)
IT **131736-68-0** 249924-28-5
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(enzymic properties of rat group IIA and V phospholipases A2 compared)
REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 9 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:423630 HCAPLUS Full-text
DOCUMENT NUMBER: 131:225307
TITLE: Novel reversible, irreversible and fluorescent inhibitors of platelet-activating factor acetylhydrolase as mechanistic probes

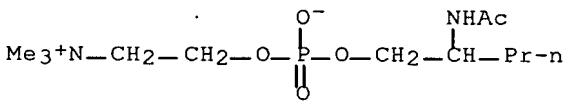
AUTHOR(S): Deigner, Hans P.; Kinscherf, Ralf; Claus, Ralf; Fyrnys, Beatrix; Blencowe, Christopher; Hermetter, A.
CORPORATE SOURCE: Pharmazeutisch-Chemisches Institut, Im Neuenheimer Feld 364, Universitat Heidelberg, Heidelberg, 69120, Germany
SOURCE: Atherosclerosis (Shannon, Ireland) (**1999**), 144(1), 79-90
CODEN: ATHSBL; ISSN: 0021-9150
PUBLISHER: Elsevier Science Ireland Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Phosphatidylcholines (1-O-alcoxy-2-amino-2-desoxy-phosphocholines and 1-pyrene-labeled analogs) were synthesized and used to examine interactions with recombinant human PAF-acetylhydrolase (PAF-AH), an enzyme purified from plasma, and with macrophage-like U937 cells. Novel phosphatidylcholines containing a sn-2-carbamoylester group such as 1-O-hexadecyl-2-desoxy-2-amino-methylcarbamoyl-2-methyl-rac-gly cero-3-phosphocholine were found to act as site-specific irreversible enzyme inhibitors with Ki-values up to 83 (Kirev) and 177 (Ki(inact)) μm. The compds. exhibit only marginal inhibition of Ca2+-dependent phospholipases. Kinetic data show that phosphocholines carrying a terminal sn-1-pyrene moiety inhibit PAF-AH activity with an effectivity similar to analogs with an aliphatic chain. 1-O-Decyloxy-[10-(4-pyrenyl)-butoxy]-2-desoxy-2-amino-carbamoyl-methyl-rac-glycero-3-phosphocholine could be used for enzyme labeling and to demonstrate an inhibitor-enzyme stoichiometry of 0.7:1. At 8°, the compound accumulated in the membranes of U937 cells, at 37° it was internalized into intracellular compartments. Structure-activity studies in a mixed micelle assay indicated that the inhibition power of reversible and irreversible inhibitors increases along with the (sn)-1-chain length similar to the structure-dependent binding of ether phospholipids to the PAF-receptor. Unlike the situation at the (sn)-1-position, increasing chain length at the sn-2-position, or an alkyl branching of the glycerol backbone significantly reduced the inhibitory potency.

IT **244013-79-4**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of novel reversible, irreversible and fluorescent inhibitors of platelet-activating factor acetylhydrolase and their interaction with enzyme and with macrophage-like U937 cells)

RN 244013-79-4 HCAPLUS

CN 3,5-Dioxa-8-aza-4-phosphadecan-1-aminium, 4-hydroxy-N,N,N-trimethyl-9-oxo-7-propyl-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



CC 7-3 (Enzymes)
Section cross-reference(s): 13, 26

IT 92445-98-2 141858-54-0 141858-55-1 141858-57-3 141858-58-4
244013-79-4
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of novel reversible, irreversible and fluorescent

inhibitors of platelet-activating factor acetylhydrolase and their interaction with enzyme and with macrophage-like U937 cells)

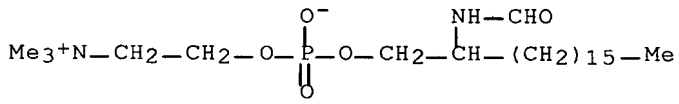
REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 10 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:380533 HCAPLUS Full-text
DOCUMENT NUMBER: 129:146164
TITLE: Inhibition of 14-kDa PLA2 by 2-acylamino-alkylphospholipids: the influence of amide acidity
AUTHOR(S): Kley, Jorg T.; Unger, Clemens; Massing, Ulrich
CORPORATE SOURCE: Tumor Biology Center, Division of Medical Research, Department of Medical Oncology, Freiburg, D-79106, Germany
SOURCE: Biochimica et Biophysica Acta, Lipids and Lipid Metabolism (**1998**), 1392(2-3), 193-201
CODEN: BBLLA6; ISSN: 0005-2760
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 2-Acylamino-alkyl phospholipids are potent competitive inhibitors of 14-kDa phospholipases A2 (e.g., human nonpancreatic secretory PLA2). As concluded from X-ray studies the amide hydrogen of these inhibitors forms a hydrogen bond to His-48 in the active site of the enzyme. We investigated the quant. contribution of this hydrogen bond to inhibition using especially designed inhibitors that bear different acyl chains with and without electron withdrawing or donating substituents, thus differing in amide acidity. Relative free enthalpies ΔΔG of enzyme-inhibitor complex formations were calculated from Xi(50) values determined by pH-stat titration using a mixed micelles assay and PLA2 from Naja mocambique mocambique. A quant. relationship between amide acidity and ΔΔG values is presented. Comparison of isoacidic and isosteric inhibitors reveals that (i) the hydrogen bond of the amide proton to His-48 is crucial for strong PLA2 inhibition, (ii) regardless of the headgroup unsubstituted N-acyl groups result in optimal amide acidity for PLA2 inhibition and (iii) the exceptionally strong inhibition by acetamides and the isosteric fluoroacetamides is due to an addnl. steric effect.

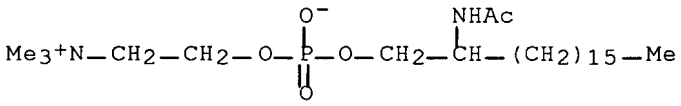
IT **210898-11-6 210898-19-4 210898-33-2 210898-51-4**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(amide acidity influence on the inhibition of 14-kDa phospholipase A2 by acylaminoalkylphospholipids)

RN 210898-11-6 HCAPLUS
CN 5,7-Dioxa-2-aza-6-phosphanonan-9-aminium, 3-hexadecyl-6-hydroxy-N,N,N-trimethyl-1-oxo-, inner salt, 6-oxide (9CI) (CA INDEX NAME)

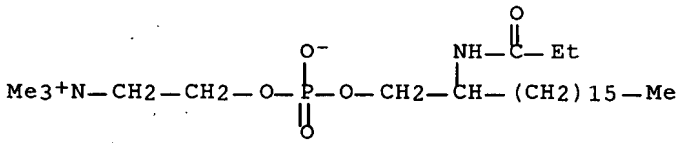


RN 210898-19-4 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphadecan-1-aminium, 7-hexadecyl-4-hydroxy-

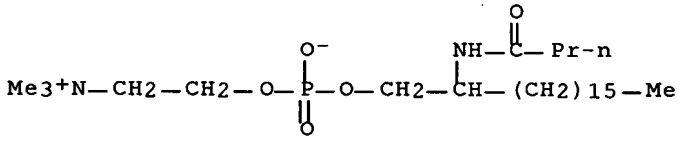
N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



RN 210898-33-2 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaundecan-1-aminium, 7-hexadecyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



RN 210898-51-4 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphadodecan-1-aminium, 7-hexadecyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



CC 7-3 (Enzymes)
IT 203178-11-4 203178-16-9 203178-17-0 203178-19-2 203178-20-5
203178-21-6 **210898-11-6 210898-19-4**
210898-24-1 210898-31-0 **210898-33-2** 210898-36-5
210898-48-9 **210898-51-4**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(amide acidity influence on the inhibition of 14-kDa phospholipase A2 by acylaminoalkylphospholipids)
REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 11 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:420028 HCAPLUS Full-text
DOCUMENT NUMBER: 127:158385
TITLE: X-ray crystal structure determination and molecular dynamics simulation of prophospholipase A2 inhibited by amide-type substrate analogs
AUTHOR(S): Tomoo, Koji; Yamane, Atsushi; Ishida, Toshimasa; Fujii, Shinobu; Ikeda, Kiyoshi; Iwama, Seiji;

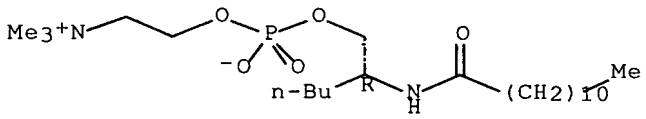
Katsumura, Shigeo; Sumiya, Shigeyuki; Miyagawa, Hiroo; Kitamura, Kunihiro
CORPORATE SOURCE: Osaka University of Pharmaceutical Sciences, 4-20-1 Nasahara, Takatsuki, Osaka, 569-11, Japan
SOURCE: Biochimica et Biophysica Acta, Protein Structure and Molecular Enzymology (**1997**), 1340(2), 178-186
CODEN: BBAEDZ; ISSN: 0167-4838
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB X-ray crystal structures of bovine pancreas prophospholipase A2 (proPLA2) inhibited by two amide-type inhibitors, [(R)-2-dodecanoyl-amino-1-hexanolphosphocholine (DAHPc) and (R)-2-dodecanoylamino-1-hexanolphosphoglycol (DAHPg)], were determined to R = 0.208 and 0.215 using reflections with up to 2.1 Å resolution, resp. Both complex crystals lacked defined electron densities for the prosequence of the N-terminal and for a loop region consisting of residues 65-70, retaining the disordered feature observed in free proPLA2 despite stabilization due to complex formation. The polar and nonpolar moieties of the amide-type inhibitors were located in the calcium-binding pocket and in the N-terminal α-helical hydrophobic region of the enzyme, resp. As for the amide group of the inhibitor, which is lacking in the true substrate, a strong hydrogen bond was formed between the NH of the inhibitor and the unprotonated Nδ1 atom of His-48, resulting in the tight binding of the inhibitor to proPLA2, as well as to PLA2. The 20-30 times more potent inhibitory activity of DAHPg than DAHPc toward PLA2 could be explained by hydrogen bond formation between the glycol OH of DAHPg and the carbonyl O of Asp-49. The seven residues of the N-terminal prosequence of proPLA2, though disordered, block the access of a water mol. to Ala-1 of PLA2 or change the hydrogen-bonding property of Ala-1 α-amino group, resulting in breakage of the water-mediated hydrogen-bond network which is commonly formed in PLA2. The results of mol. dynamics (MD) calcn. in an aqueous solution at 300 K indicate that this, rather than the close contact between the prosequence and the residues 65-70 loop region, is the main reason why the latter region becomes flexible in proPLA2, compared with in PLA2.

IT **131736-68-0**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(X-ray crystal structure determination and mol. dynamics simulation of prophospholipase A2 inhibited by amide-type substrate analogs)

RN 131736-68-0 HCAPLUS

CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 7-5 (Enzymes)
Section cross-reference(s): 75

IT 7440-70-2, Calcium, biological studies **131736-68-0**
136134-09-3
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological

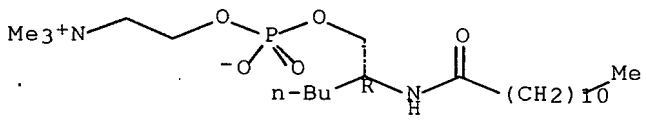
study)
(X-ray crystal structure determination and mol. dynamics simulation of prophospholipase A2 inhibited by amide-type substrate analogs)
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 12 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:887283 HCAPLUS Full-text
DOCUMENT NUMBER: 124:116942
TITLE: New phospholipase A2 inhibitor: synthesis and inhibition mechanism of oxazolidinone phospholipid analog
AUTHOR(S): Iwama, Seiji; Matsuda, Takeshi; Katsumura, Shigeo; Tani, Takeshi; Fujii, Shinobu; Ikeda, Kiyoshi; Takehara, Hideki
CORPORATE SOURCE: Sch. Sci., Kwansei Gakuin Univ., Nishinomiya, 662, Japan
SOURCE: Bioorganic & Medicinal Chemistry (**1995**), 3(10), 1397-403
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB (R)-2-[[hydroxy[[2-oxo-3-(1-oxododecyl)-4- oxazolidinyl]methoxy]phosphinyl]oxy]-N,N,N-trimethylethanaminium inner salt [i.e., (R)-dodecanoyl-4-phosphatidylcholino(hydroxymethyl)-2-oxazolidinone] (I), which is a new glycerophospholipid analog, was synthesized starting from (S)-glycidol through a 4-alkylsilyloxymethyl derivative and N-acyl-4-hydroxymethyl derivative The cyclic amide analog of I showed strong inhibitory activity toward both Group I and II PLA2s, but the inhibitory potency of I was slightly weaker than that of the linear amide analog (R)-7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-3,5-dioxa-8-aza-4-phosphaeicosan-1-aminium 4-oxide inner salt (II), which had been developed by de Haas et al. (Biochem. Biophys. Acta 1990, 1043, 67). The interactions of I with human secretory PLA2 was investigated by computer modeling in comparison with those of the linear amide analog II. The results of the computer modeling were very compatible with those of the inhibitory activities toward PLA2s, and the both results showed that the binding mode of the oxazolidinone analog I was very similar to that of the genuine substrate and was different from that of the linear amide analog II.

IT **131736-68-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and inhibition mechanism of oxazolidinone phospholipid analog as phospholipase A2 inhibitor)
RN 131736-68-0 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (7R)- (9CI) (CA INDEX NAME)

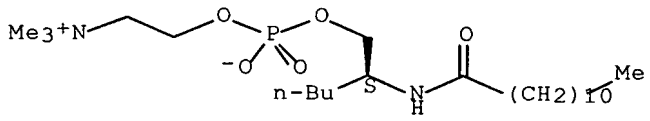
Absolute stereochemistry.



IT **131736-67-9P**, 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium,

7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (S)
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and inhibition mechanism of oxazolidinone phospholipid analog as phospholipase A2 inhibitor)
RN 131736-67-9 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 26-9 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1, 28
IT **131736-68-0P** 155398-64-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and inhibition mechanism of oxazolidinone phospholipid analog as phospholipase A2 inhibitor)
IT **131736-67-9P**, 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (S) 153531-48-7P 154669-49-5P 155398-63-3P 158249-50-4P 172792-95-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and inhibition mechanism of oxazolidinone phospholipid analog as phospholipase A2 inhibitor)

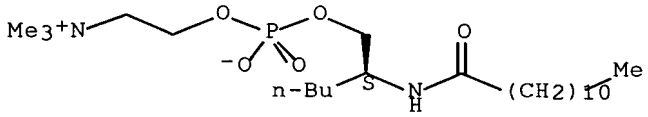
L49 ANSWER 13 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:404591 HCAPLUS Full-text
DOCUMENT NUMBER: 122:309528
TITLE: Binding mode of phospholipase A2 with a new type of phospholipid analog having an oxazolidinone ring
AUTHOR(S): Tani, Takeshi; Fujii, Shinobu; Inoue, Seiji; Ikeda, Kiyoshi; Iwama, Seiji; Matsuda, Takeshi; Katsumura, Shigeo; Samejima, Yuji; Hayashi, Kyozo
CORPORATE SOURCE: Department Biochemistry, Osaka University Pharmaceutical Sciences, Osaka, 580, Japan
SOURCE: Journal of Biochemistry (Tokyo) (**1995**), 117(1), 176-82
CODEN: JOBIAO; ISSN: 0021-924X
PUBLISHER: Japanese Biochemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Inhibition of phospholipases A2 (PLA2s) by a new type of monodispersed phospholipid analog, 3-dodecanoyl-4- phosphatidylcholinohydroxymethyl-2-oxazolidinone (oxazolidinone-PC), was investigated by the pH stat assay method using monodispersed 1,2-dihexanoyl-sn-glycero-3-phosphorylcholine (diC6PC) as the substrate. The PLA2s used were those from bovine pancreas and cobra (Naja naja atra) venom (Group I) and from Japanese mamushi (Agkistrodon halys blomhoffii) venom (Group II). This new-type substrate analog was shown to inhibit

competitively both types of venom and bovine pancreatic enzymes by binding to the active site in a similar manner to the carboxamide-type analog 2-dodecanoyl-amino-1- hexanol-phosphocholine (amide-PC). The binding of a stereoisomer, (R)-amide-PC, to N. naja atra (Group I) and A. halys blomhoffii (Group II) PLA2s was facilitated by the binding of Ca2+ to the enzymes. On the other hand, the binding of (R)-oxazolidinone-PC to the N. naja atra (Group I) enzyme was found to be independent of Ca2+ binding, while its binding to the A. halys blomhoffii (Group II) enzyme was markedly facilitated by the binding of (R)-oxazolidinone-PC was found to be practically independent of the ionization state of this residue. The Ca2+ dependency and participation of the catalytic group His 48 in the binding of genuine substrate to both types of PLA2s were found to be very similar to those for the oxazolidinone-PC, but differed greatly from those for the amide-PC, indicating that the binding mode of oxazolidinone-PC is very similar to that of the genuine substrate, but very different from that of the amide-PC.

IT **131736-67-9 131736-68-0**
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(amide phospholipid analog; binding mode of phospholipase A2 with a new type of oxazolidinone ring-containing phospholipid analog)

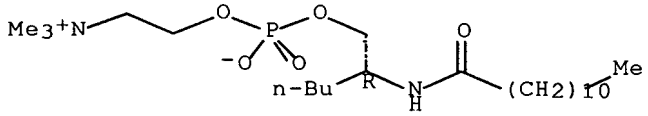
RN 131736-67-9 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 131736-68-0 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 7-3 (Enzymes)

IT **131736-67-9 131736-68-0**
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(amide phospholipid analog; binding mode of phospholipase A2 with a new type of oxazolidinone ring-containing phospholipid analog)

L49 ANSWER 14 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:557330 HCAPLUS Full-text
DOCUMENT NUMBER: 121:157330
TITLE: Synthesis of enantiomerically pure 1-O-phosphocholine-2-O-acyl-octadecane and

1-O-phosphocholine-2-N-acyl-octadecane

AUTHOR(S): Massing, Ulrich; Eibl, Hansjoerg
CORPORATE SOURCE: Membrane Biophys., Max Planck Inst. Biophys. Chem., Goettingen, 37077, Germany

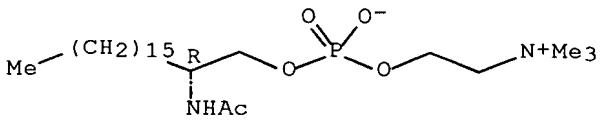
SOURCE: Chemistry and Physics of Lipids (**1994**), 69(2), 105-20
CODEN: CPLIA4; ISSN: 0009-3084
DOCUMENT TYPE: Journal
LANGUAGE: English

AB This is the first report on the chemical synthesis of enantiomerically pure R- or S-1-O-phosphocholine-2-O-acyloctadecanes, Me3N+CH2CH2OP(O)(O-)OCH2CH(XCOR)CH2CH2(CH2)11Pr (I, R = Me, C11H23, C15H31, C17H35, C17H37, X = O) and R- or S-1-O-phosphocholine-2-N- acyl-octadecanes I (X = NH). From a structural point of view these phospholipids are intermediates between phosphatidylcholine and sphingomyelin. The synthesis of these model compds. is based on R- or S-1,2-O-isopropylidene-glyceraldehyde for chain elongation in a Wittig reaction with pentadecanetriphenylphosphine bromide. The resulting 1,2-O-isopropylidene-octadec-3-ene is converted to R- or S-1,2-octadecanediol by catalytic hydrogenation of the double bond and by acidic removal of the isopropylidene protecting group. Tritylation of R- or S-1,2-octadecanediol results in the general intermediates R- or S-1-O-trityl-2-hydroxyoctadecane. These are the key intermediates for the synthesis of the phosphatidylcholine- or sphingomyelin-like end products. R- or S-1-O-phosphocholine-2-O- acyl-octadecane is obtained from the tritylated intermediates via benzylation in position 2, acidic detritylation and conversion of the R- or S-1-hydroxy-2-benzyl-octadecanes to the resp. phosphocholines via the phosphoethanolamines. Catalytic hydrogenolysis of the benzyl group results in R- or S-1-O-phosphocholine-2-hydroxy-octadecane, which is converted to the phosphatidylcholine-like end products by acylation. R- or S-1-O-phosphocholine-2-N-acyl-octadecane is obtained from the tritylated intermediate by conversion of the R- or S-2-hydroxy group into the N-phthalimido group, which is achieved by inversion of the configuration using the Mitsunobu reaction with phthalimide. After acidic detritylation, the product is converted to the resp. S- or R-1-O-phosphocholine derivative in a similar sequence of reactions. The phthalimido group is converted to the 2-amino group, and acylation results in the sphingomyelin-like end products.

IT **156991-49-0P 156991-50-3P 156991-51-4P**
156991-58-1P 156991-59-2P 156991-60-5P
157086-02-7P 157086-03-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

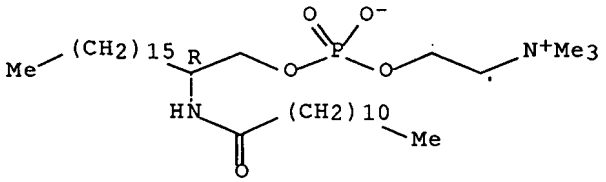
RN 156991-49-0 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphadecan-1-aminium, 7-hexadecyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



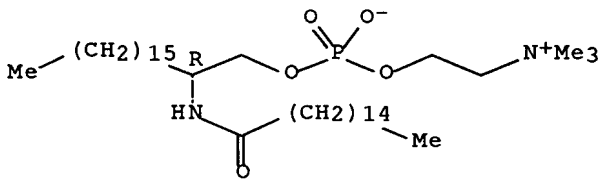
RN 156991-50-3 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 7-hexadecyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



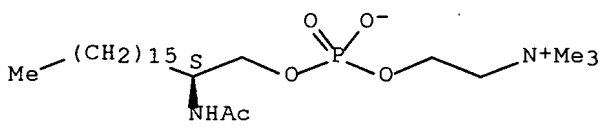
RN 156991-51-4 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphatetracosan-1-aminium, 7-hexadecyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



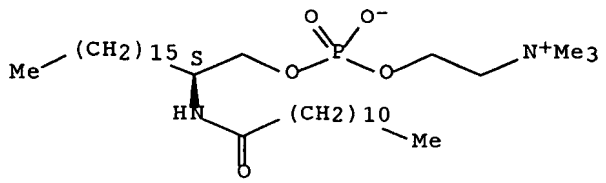
RN 156991-58-1 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphadecan-1-aminium, 7-hexadecyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (7S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 156991-59-2 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 7-hexadecyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (S)- (9CI) (CA INDEX NAME)

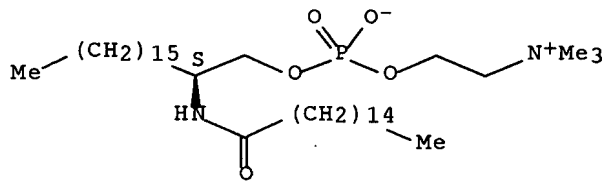
Absolute stereochemistry.



RN 156991-60-5 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphatetracosan-1-aminium, 7-hexadecyl-4-hydroxy-

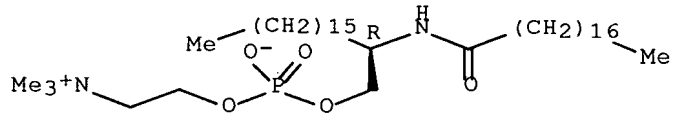
N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



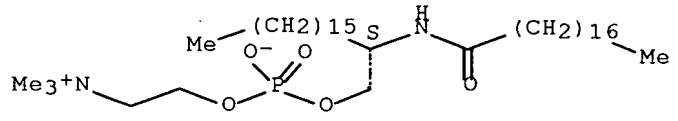
RN 157086-02-7 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphahexacosan-1-aminium, 7-hexadecyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 157086-03-8 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphahexacosan-1-aminium, 7-hexadecyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 26-3 (Biomolecules and Their Synthetic Analogs)
IT 156991-44-5P 156991-45-6P 156991-46-7P 156991-47-8P
156991-48-9P **156991-49-0P 156991-50-3P**
156991-51-4P 156991-52-5P 156991-53-6P 156991-54-7P
156991-55-8P 156991-56-9P 156991-57-0P **156991-58-1P**
156991-59-2P 156991-60-5P 156991-61-6P
157086-02-7P 157086-03-8P 157394-07-5P
157394-08-6P 157394-09-7P 157394-10-0P 157394-11-1P
157394-12-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L49 ANSWER 15 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:534457 HCAPLUS Full-text
DOCUMENT NUMBER: 121:134457
TITLE: Preparation of phosphatidylcholine analogs as phospholipase A2 inhibitors

INVENTOR(S): Eibl, Hansjoerg; Massing, Ulrich; Unger, Clemens
PATENT ASSIGNEE(S): Max-Planck-Gesellschaft zur Foerderung der Wissenschaften e.V., Germany
SOURCE: Ger. Offen., 15 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4234130	A1	19940414	DE 1992-4234130	19921009
WO 9409014	A1	19940428	WO 1993-EP2762	19931008

W: AT, AU, BB, BG, BR, BY, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, US, VN
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

AU 9351500	A	19940509	AU 1993-51500	19931008
EP 663918	A1	19950726	EP 1993-922534	19931008

R: AT, BE, CH, DE, DK, ES, FR, GB, IE, IT, LI, NL, SE

JP 08502735	T	19960326	JP 1993-509591	19931008

PRIORITY APPLN. INFO.:	DE 1992-4234130 A	19921009
	WO 1993-EP2762 W	19931008

OTHER SOURCE(S): CASREACT 121:134457; MARPAT 121:134457

AB R1R2CHCH2OR [R = P(O)(O-)OCH2CH2N+Me3] (I; R1 = C10-22 alkyl; R2 = O2CR3, NHCOR3; R3 = C1-20 alkyl) were prepared Addnl. claimed were ROCHR1CH2R2. Thus, (R)-I (R1 = hexadecyl, R2 = NHAc), prepared in 7 steps from O,O-(isopropylidene)glyceraldehyde, gave 100% inhibition of phospholipase A2 at 10% the concentration of dipalmitoyllecithin substrate.

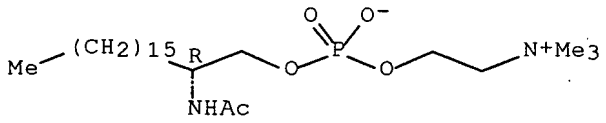
IT **156991-49-0P 156991-50-3P 156991-51-4P 156991-58-1P 156991-59-2P 156991-60-5P 157086-02-7P 157086-03-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of, as phospholipase A2 inhibitor)

RN 156991-49-0 HCAPLUS

CN 3,5-Dioxa-8-aza-4-phosphadecan-1-aminium, 7-hexadecyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (7R)- (9CI) (CA INDEX NAME)

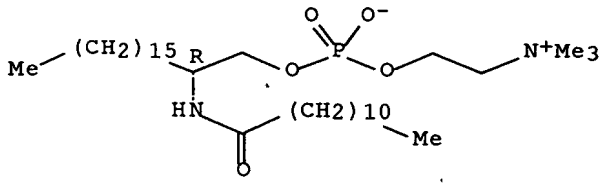
Absolute stereochemistry.



RN 156991-50-3 HCAPLUS

CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 7-hexadecyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

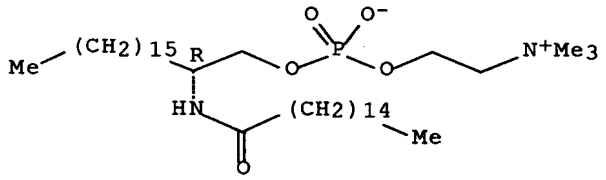
Absolute stereochemistry.



RN 156991-51-4 HCAPLUS

CN 3,5-Dioxa-8-aza-4-phosphatetracosan-1-aminium, 7-hexadecyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

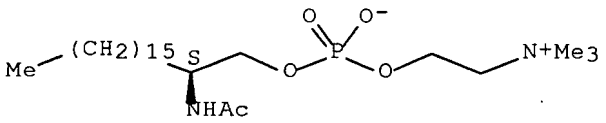
Absolute stereochemistry.



RN 156991-58-1 HCAPLUS

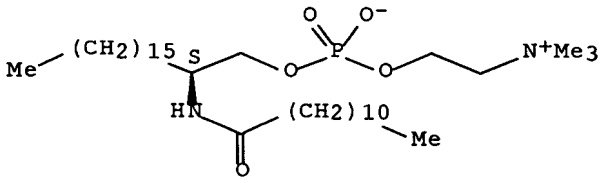
CN 3,5-Dioxa-8-aza-4-phosphadecan-1-aminium, 7-hexadecyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (7S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



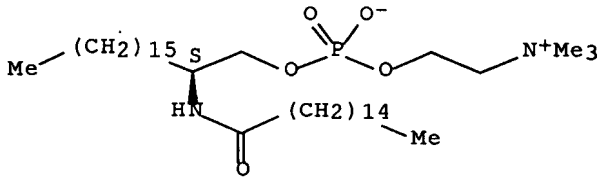
RN 156991-59-2 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 7-hexadecyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



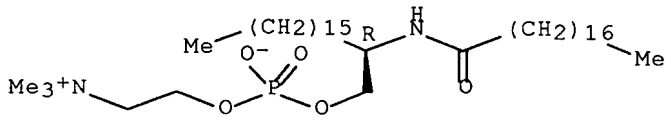
RN 156991-60-5 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphatetracosan-1-aminium, 7-hexadecyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



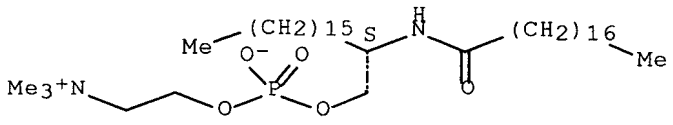
RN 157086-02-7 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphahexacosan-1-aminium, 7-hexadecyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 157086-03-8 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphahexacosan-1-aminium, 7-hexadecyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07F009-10
ICS A61K031-685; C12N009-99; C12N009-16
CC 29-6 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 1
IT 156991-44-5P 156991-45-6P 156991-46-7P 156991-47-8P
156991-48-9P **156991-49-0P 156991-50-3P**
156991-51-4P 156991-52-5P 156991-53-6P 156991-54-7P
156991-55-8P 156991-56-9P 156991-57-0P **156991-58-1P**
156991-59-2P 156991-60-5P 156991-61-6P
157086-02-7P 157086-03-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as phospholipase A2 inhibitor)

L49 ANSWER 16 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:528471 HCAPLUS Full-text
DOCUMENT NUMBER: 121:128471
TITLE: Competitive inhibition of lipolytic enzymes. X. Further delineation of the active site of pancreatic phospholipases A2 from pig, ox and horse by comparing the inhibitory power of a number of (R)-2-acylamino phospholipid analogs
AUTHOR(S): Dijkman, R.; Cox, R.; Berg, L. van den; Verheij, H. M.; Haas, G. H. De
CORPORATE SOURCE: Department of Enzymology and Protein Engineering, C.B.L.E., Padualaan 8, CH Utrecht, 3584, Neth.
SOURCE: Biochimica et Biophysica Acta, Lipids and Lipid Metabolism (**1994**), 1212(1), 50-8
CODEN: BBLLA6; ISSN: 0005-2760
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

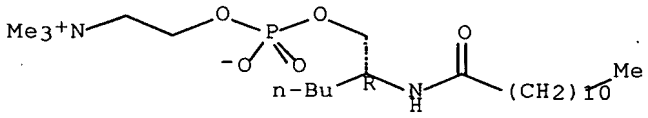
AB Two series of (R)-phospholipid analogs, each containing a n-Pr group at the C-1 position and various acylamino functions at the C-2 position have been synthesized and their inhibitory properties towards three mammalian pancreatic phospholipases A2 have been determined The members of the first series of analogs all contained the zwitter-ionic phosphocholine headgroup which in the second series was replaced by the anionic phosphoglycol function. In the saturated 2-acylamino phospholipids the length of the acyl chain ranged from 8 to 18 carbon atoms. The unsatd. 2-acylamino analogs possessed a chain length of 11 or 18 carbon atoms and contained one, two, three or four double bonds. For inhibitors with a saturated acylamino group, the phospholipases A2 from pig, ox and horse show a sharp optimum in inhibitory power Z for an acyl chain length of 10 carbon atoms. The inhibitory behavior of the unsatd. acylamino analogs is more complex: both the zwitter-ionic and the anionic inhibitors demonstrate an increase in Z with an increasing number of cis-double bonds but the degree of improvement is dependent on the position of the double bonds. Subsequently the influence of polar groups at carbon position 12 of the dodecanoylamino phospholipids on Z was analyzed. Substitution of the

terminal Me group by an OH-function lowers the inhibitory potency of the three enzymes by a factor of 4 to 5 both in the phosphocholine and phosphoglycol series. Replacement of the Me group by potentially charged functions (-NH2, -COOH) resulted in a complete loss of inhibitory properties. Blocking of the amino group and carboxyl function by t-butyloxycarbonylation and esterification, resp., fully restored the inhibitory power. Finally the authors investigated how changes in the polar headgroup and the presence of aromatic rings at the C-1 or C-2 position influenced the inhibitory potency of the analogs.

IT **131736-68-0 131736-76-0 131736-77-1**
131736-79-3 157057-53-9 157057-54-0
157057-55-1 157057-56-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phospholipase A2 of horse and ox and pig, structure in relation to)

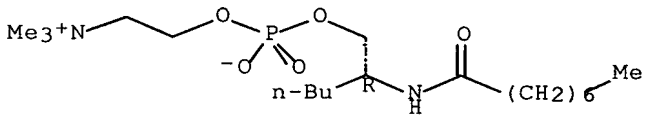
RN 131736-68-0 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



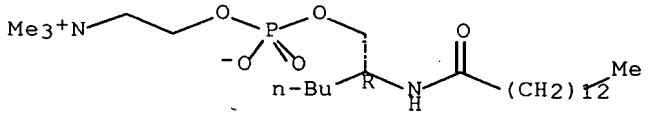
RN 131736-76-0 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphahexadecan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



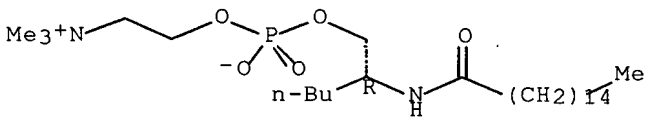
RN 131736-77-1 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphadocosan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



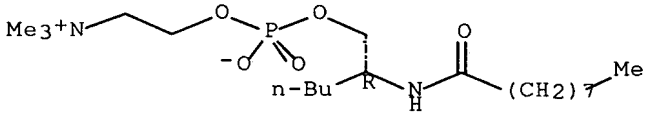
RN 131736-79-3 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphatetracosan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



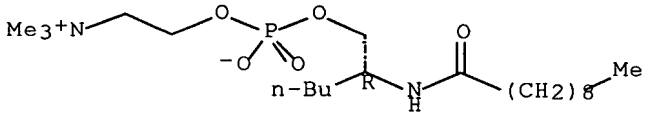
RN 157057-53-9 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaheptadecan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



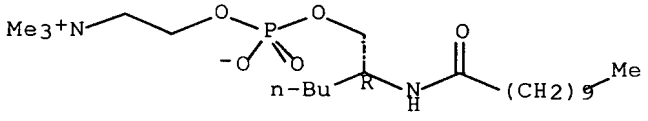
RN 157057-54-0 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaoctadecan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



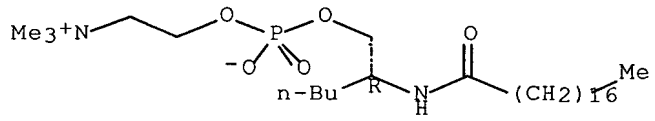
RN 157057-55-1 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphanonadecan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 157057-56-2 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphahexacosan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

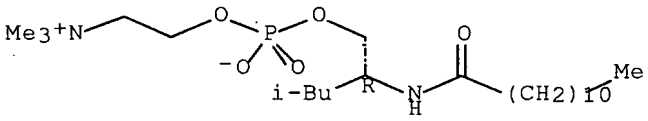
Absolute stereochemistry.



CC 7-3 (Enzymes)
Section cross-reference(s): 13
IT **131736-68-0 131736-76-0 131736-77-1**
131736-78-2 **131736-79-3** 131736-80-6 131764-78-8
136134-09-3 146426-17-7 146426-18-8 146426-19-9 146565-08-4
149002-93-7 149002-94-8 **157057-53-9 157057-54-0**
157057-55-1 157057-56-2 157057-57-3
157057-58-4 157057-59-5 157057-60-8 157057-61-9 157057-62-0
157057-63-1 157057-64-2 157057-65-3 157057-66-4 157057-67-5
157057-68-6 157057-69-7 157057-70-0 157057-71-1 157057-72-2
157057-73-3 157057-74-4 157057-75-5 157057-76-6 157057-77-7
157057-78-8 157057-79-9 157057-80-2 157057-81-3 157057-82-4
157057-83-5 157057-84-6 157057-85-7 157057-86-8 157057-87-9
157057-88-0 157057-89-1 157057-90-4 157057-91-5 157057-92-6
157057-93-7 157182-46-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phospholipase A2 of horse and ox and pig, structure in relation to)

L49 ANSWER 17 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:502736 HCAPLUS Full-text
DOCUMENT NUMBER: 121:102736
TITLE: NMR and IR studies of the effect of calcium on the binding of inhibitors to phospholipase A2
AUTHOR(S): Slaich, P. K.; Primrose, W. U.; Robinson, D. H.; Wharton, C. W.; White, A. J.; Drabble, K.; Roberts, G. C. K.
CORPORATE SOURCE: Biol. NMR Cent., Univ. Leicester, Leicester, UK
SOURCE: Int. Conf. Spectrosc. Biol. Mol., 5th (**1993**), 241-3. Editor(s): Theophanides, Theophile; Anastassopoulou, Jane; Fotopoulos, Nikolaos. Kluwer: Dordrecht, Neth.
CODEN: 60ABAD
DOCUMENT TYPE: Conference
LANGUAGE: English
AB NMR and IR studies of the binding of an inhibitory amide analog of a phospholipase A2 substrate were carried out. In the analog, an amide group is placed at the site where and ester bond would normally be cleaved. The effects of calcium and Gly-30 can be approximated to that of one extra H bond to the carbonyl O atom in the enzyme complex.
IT **131736-69-1**
RL: BIOL (Biological study)
(phospholipase A2 inhibition by, calcium effect on)
RN 131736-69-1 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-7-(2-methylpropyl)-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

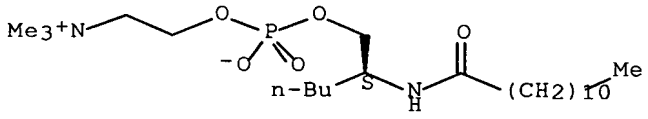
Absolute stereochemistry.



CC 7-3 (Enzymes)
IT **131736-69-1**
RL: BIOL (Biological study)
(phospholipase A2 inhibition by, calcium effect on)

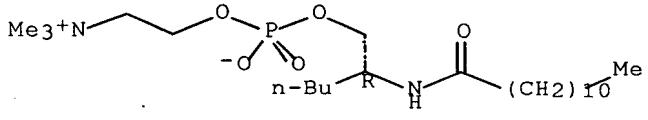
L49 ANSWER 18 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:315158 HCAPLUS Full-text
DOCUMENT NUMBER: 120:315158
TITLE: Synthesis of oxazolidinone phospholipid analog as a new inhibitor of phospholipase A2
AUTHOR(S): Katsumura, Shigeo; Iwama, Seiji; Matsuda, Takeshi; Tani, Takeshi; Fujii, Shinobu; Ikeda, Kiyoshi
CORPORATE SOURCE: Fac. Sci., Kwansei Gakuin Univ., Nishinomiya, 662, Japan
SOURCE: Bioorganic & Medicinal Chemistry Letters (**1993**), 3(12), 2703-6
CODEN: BMCLE8; ISSN: 0960-894X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB (S)- and (R)-3-dodecanoyl-4-phosphatidylcholinoxymethyl-2- oxazolidinone, which are cyclic analogs of the amide phospholipid C11H23CONHCHBuCH2OP(O)(O-)OCH2CH2N+Me3 (I), were synthesized. The inhibitory activities of these analogs toward phospholipase A2 were compared with that of the amide analog I.
IT **131736-67-9 131736-68-0**
RL: BIOL (Biological study)
(phospholipase A2 inhibition by)
RN 131736-67-9 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 131736-68-0 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (7R)- (9CI) (CA INDEX NAME)

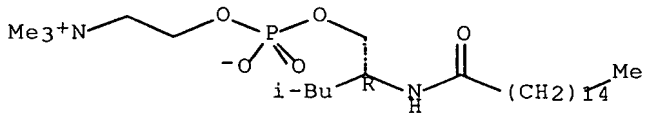
Absolute stereochemistry.



CC 1-3 (Pharmacology)
Section cross-reference(s): 28
IT **131736-67-9 131736-68-0**
RL: BIOL (Biological study)
(phospholipase A2 inhibition by)

L49 ANSWER 19 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:238899 HCAPLUS Full-text
DOCUMENT NUMBER: 120:238899
TITLE: Discovery of new non-phospholipid inhibitors of the secretory phospholipases A2
AUTHOR(S): Beaton, Haydn G.; Bennion, Colin; Connolly, Stephen; Cook, Anthony R.; Gensmantel, Nigel P.; Hallam, Catherine; Hardy, Kim; Hitchin, Barbara; Jackson, Clive G.; Robinson, David H.
CORPORATE SOURCE: Pharmaceutical Division, Fisons PLC, Loughborough/Leicestershire, LE11 ORH, UK
SOURCE: Journal of Medicinal Chemistry (**1994**), 37(5), 557-9
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Anal. of the binding interactions (previously determined by 2D NMR and mol. modeling techniques) between pancreatic phospholipase A2 and substrate-like phospholipid inhibitors has led to the design of a novel series of nonphospholipid analogs which demonstrate high levels of inhibitory activity against both the porcine pancreatic and human platelet secreted enzymes. A crucial feature of the design involved the replacement of the phosphocholine moiety present in the early inhibitors by a simple carboxylic acid group. The study provides one of the first examples of the successful use of the carboxylic acid function as a bioisosteric replacement for a phosphodiester group in the rational design of biol. active mols.
IT **142003-37-0**
RL: BIOL (Biological study)
(phospholipase A2 of pancreas and human platelets inhibition by, structure in relation to)
RN 142003-37-0 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphatetracosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-7-(2-methylpropyl)-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 7-3 (Enzymes)
IT 56217-80-2 136702-50-6 136702-73-3 136703-04-3 136703-18-9 136703-36-1 **142003-37-0** 154414-48-9 154414-49-0 154414-50-3 154414-51-4 154414-52-5 155279-59-7
RL: BIOL (Biological study)
(phospholipase A2 of pancreas and human platelets inhibition by, structure in relation to)

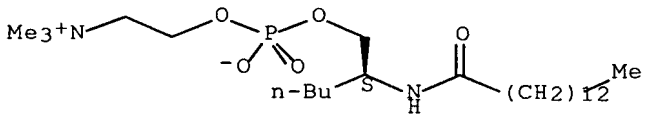
L49 ANSWER 20 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1993:554708 HCAPLUS Full-text
DOCUMENT NUMBER: 119:154708
TITLE: Stereospecificity of the interaction of porcine pancreatic phospholipase A2 with micellar and monomeric inhibitors. A time-resolved fluorescence study of the tryptophan residue
AUTHOR(S): Vincent, Michel; Deveer, Anne Mieke; De Haas, Gerard H.; Verheij, Hubertus M.; Gallay, Jacques
CORPORATE SOURCE: Lab. Util. Rayonnem. Electromagn., Univ. Paris-Sud, Orsay, F-91405, Fr.
SOURCE: European Journal of Biochemistry (**1993**), 215(3), 531-9
CODEN: EJBCAI; ISSN: 0014-2956
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The effect of binding enantiomeric substrate analogs in micellar form on the local conformation and dynamics of the N-terminal region of porcine pancreas phospholipase A2 was examined by time-resolved fluorescence measurements of its single tryptophan residue (Trp3). The complexity of the fluorescence intensity decay of the unliganded protein (four excited-state lifetime populations) suggests conformational heterogeneity in the N-terminal region of the protein. A considerable simplification of the excited-state lifetime profile was observed in the complex with one of the stereoisomers [(R)-2-tetradecanoylamino)-hexanol-phosphocholine] at a low inhibitor/protein molar ratio (≈9). This indicates the existence of a definite conformation of the N-terminal region of the protein in the complex. No effect was detected for the S-enantiomer. In parallel, the rotational mobility of the Trp residue in the complex with the R-enantiomer was reduced. At a higher inhibitor/protein molar ratio of ≈130, the stereospecificity of the interaction was lost and complexes were formed with both stereoisomers. These complexes, however, differed from the specific one in terms of the local Trp3 environment and the volume of the rotating unit. The local effects of low amts. of monomeric inhibitors added to a preformed protein/micelle complex of a phospholipase A2 double mutant in which a Trp residue was genetically inserted near the active site at position 31 while the natural Trp3 was replaced by Phe (Kuipers, O., et al., 1991), were also monitored by time-resolved fluorescence. A stereospecific dependence of the local perturbations was again observed These results support the idea that the active conformation of the protein is reached in solution only after formation of a ternary complex, protein-interface-inhibitor.

IT **143554-25-0**
RL: BIOL (Biological study)
(binding of, by phospholipase A2, enzyme conformation and mobility response to)
RN 143554-25-0 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphadocosan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (S)- (9CI) (CA INDEX NAME)

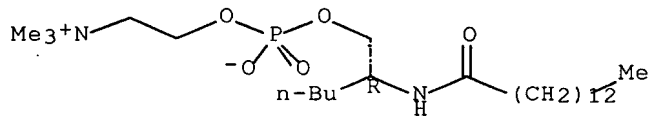
Absolute stereochemistry.



IT **131736-77-1**
RL: BIOL (Biological study)
(binding of, by phospholipase A2, enzyme conformation response to, stereospecificity in relation to)

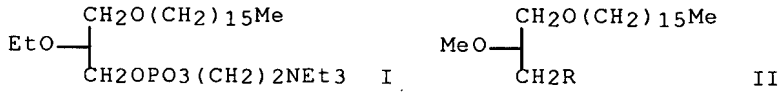
RN 131736-77-1 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphadocosan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 7-3 (Enzymes)
IT 58066-85-6, n-Hexadecylphosphocholine 131736-78-2 142629-54-7 **143554-25-0**
RL: BIOL (Biological study)
(binding of, by phospholipase A2, enzyme conformation and mobility response to)
IT **131736-77-1**
RL: BIOL (Biological study)
(binding of, by phospholipase A2, enzyme conformation response to, stereospecificity in relation to)

L49 ANSWER 21 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1993:539633 HCAPLUS Full-text
DOCUMENT NUMBER: 119:139633
TITLE: Synthesis of phosphocholine and quaternary amine ether lipids and evaluation of in vitro antineoplastic activity
AUTHOR(S): Morris-Natschke, Susan L.; Gumus, Fatma; Marasco, Canio J., Jr.; Meyer, Karen L.; Marx, Michael; Piantadosi, Claude; Layne, Matthew D.; Modest, Edward J.
CORPORATE SOURCE: Sch. Pharm., Univ. North Carolina, Chapel Hill, NC, 27599, USA
SOURCE: Journal of Medicinal Chemistry (**1993**), 36(14), 2018-25
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

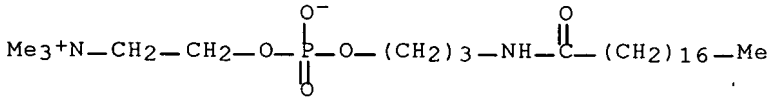


AB The in vitro antineoplastic activity of phosphocholines, e.g. I, and quaternary amine ether lipids, e.g. II (R = 3- hydroxymethylpyridinium bromide), has been evaluated in the HL-60 promyelocytic cell line. These compds. are analogs of ET-18-OMe (1-O-octadecyl-2-O-methyl-rac-glycero-3-phosphocholine). Structural modification of 1-(alkylamido)-, -(alkylthio)-, and -(alkyloxy)propyl backbones has provided further insight into the structure-activity relationships of these lipids. In this study, a long saturated C-1 chain and a three-carbon backbone with a single short C-2 substituent were preferred. At the pos. charged nitrogen

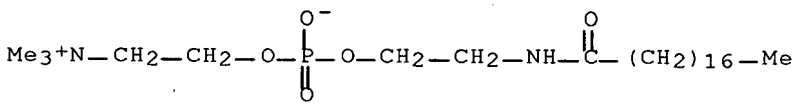
of phosphocholines, fewer than three substituents caused a significant loss of activity, and substituents larger than Me decreased activity slightly. In the nonphosphorus compds., many nitrogen heterocycles and also a sulfonium moiety were incorporated without changing the degree of activity; however, a thiazolium group decreased activity. II was approx. twice as active as the reference standard, ET-18-OMe, in a trypan blue dye exclusion assay.

IT **76506-75-7P 82755-92-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antitumor activity of)

RN 76506-75-7 HCAPLUS
CN 3,5-Dioxa-9-aza-4-phosphaheptacosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-10-oxo-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



RN 82755-92-8 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphahexacosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



CC 33-6 (Carbohydrates)
Section cross-reference(s): 1, 6

IT **76506-75-7P 82755-92-8P** 128723-54-6P
131730-55-7P 131933-53-4P 131933-54-5P 139574-76-8P
149576-08-9P 149576-09-0P 149576-10-3P 149576-11-4P
149576-12-5P 149576-13-6P 149576-14-7P 149576-15-8P
149576-16-9P 149576-17-0P 149576-18-1P 149576-19-2P
149576-20-5P 149576-21-6P 149576-23-8P 149576-24-9P
149576-25-0P 149576-26-1P 149576-27-2P 149576-28-3P
149576-29-4P 149576-30-7P 149576-31-8P 149576-32-9P
149576-33-0P 149576-34-1P 149576-35-2P 149576-36-3P
149576-37-4P 149576-38-5P 149656-31-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antitumor activity of)

L49 ANSWER 22 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1993:466306 HCAPLUS Full-text
DOCUMENT NUMBER: 119:66306
TITLE: Competitive inhibition of lipolytic enzymes. IX. A comparative study on the inhibition of pancreatic phospholipases A2 from different sources by (R)-2-acylamino phospholipid analogs

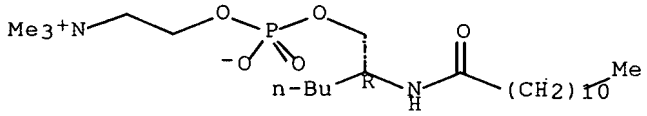
AUTHOR(S): de Haas, G. H.; Dijkman, R.; Lugtigheid, R. B.; Dekker, N.; Van den Berg, L.; Egmond, M. R.; Verheij, H. M.
CORPORATE SOURCE: Department of Enzymology and Protein Engineering, C.B.L.E., Utrecht, Neth.
SOURCE: Biochimica et Biophysica Acta, Lipids and Lipid Metabolism (**1993**), 1167(3), 281-8
CODEN: BBLLA6; ISSN: 0005-2760
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The inhibitory power (Z) of a number of (R)-1-alkyl-2-acylamino phospholipid analogs was determined for three mammalian phospholipases A2 from pig, ox and horse pancreas. All three enzymes display a clear preference for anionic (phosphoglycol) inhibitors over the zwitterionic (phosphocholine) derivs.; this effect is most pronounced for the bovine enzyme. Upon variation of the 1-alkyl chain length, the bovine and equine phospholipases, like the porcine enzyme in previous studies, show an optimum in Z for a six-carbon alkyl group. The introduction of a double bond in the 2-acylamino group generally improves the inhibitory power as compared with a fully saturated acyl chain. For the horse enzyme, the presence of an (R)-2-undecenoylamino group in the phosphocholine- and phosphoglycol-containing inhibitors resulted in affinities which are nearly 4 and 5 orders of magnitude higher, resp., than for the substrate mol. Direct determination of the dissociation constant Ki* of several inhibitors incorporated in a host lipid/water interface of noninhibitory n-octadecenylphosphocholine micelles, was performed by UV difference spectroscopy. The progressive binding of a single inhibitor mol. into the active site of the three enzymes was followed quant. by an increasing tyrosine perturbation. With moderately strong competitive inhibitors (Z values ranging from about 50 to 10,000), quant. values for Ki* were obtained. Extrapolation of the exptl. found linear relationship between Z and 1/Ki* yields predicted Ki* nos. for the much stronger inhibitors with Z values between 10,000 and 100,000.

IT **131736-68-0 131736-71-5 131736-76-0 131736-77-1 131736-79-3**
RL: BIOL (Biological study)
(phospholipase A2 of mammalian pancreas inhibition by, kinetics of, structure in relation to)

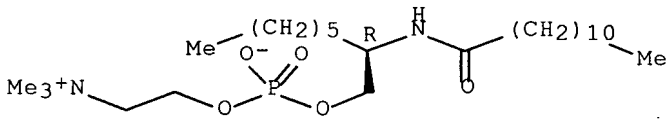
RN 131736-68-0 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



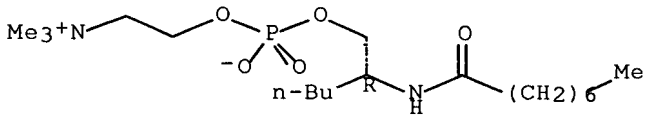
RN 131736-71-5 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 7-hexyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



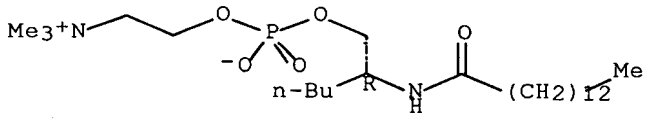
RN 131736-76-0 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphahexadecan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



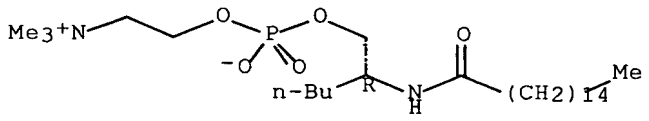
RN 131736-77-1 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphadocosan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 131736-79-3 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphatetracosan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 7-3 (Enzymes)
IT **131736-68-0 131736-71-5 131736-76-0**
131736-77-1 131736-78-2 **131736-79-3**
131736-80-6 131764-78-8 136134-09-3 141056-44-2 146426-18-8
146565-08-4 149002-93-7 149002-94-8 149002-95-9 149002-96-0
149002-97-1 149002-98-2
RL: BIOL (Biological study)
(phospholipase A2 of mammalian pancreas inhibition by, kinetics of, structure in relation to)

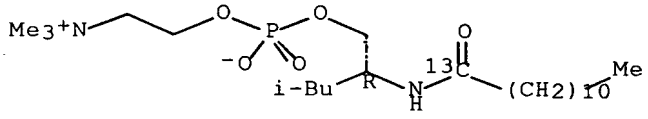
L49 ANSWER 23 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1993:18380 HCAPLUS Full-text
DOCUMENT NUMBER: 118:18380
TITLE: The binding of amide substrate analogs to phospholipase A2. Studies by carbon-13 nuclear magnetic resonance and infrared spectroscopy
AUTHOR(S): Slaich, Pritpal K.; Primrose, William U.; Robinson, David H.; Wharton, Christopher W.; White, Andrew J.; Drabble, Kevin; Roberts, Gordon C. K.
CORPORATE SOURCE: Dep. Biochem., Univ. Leicester, Leicester, LE1 9HN, UK
SOURCE: Biochemical Journal (**1992**), 288(1), 167-73
CODEN: BIJOAK; ISSN: 0306-3275
DOCUMENT TYPE: Journal
LANGUAGE: English

AB (R)-(2-Dodecanamidoisohexyl)phosphocholine (DAHPC), labeled with 13C at the amide carbonyl group, has been synthesized and its binding to bovine pancreatic phospholipase A2 (PLA2) studied by NMR and IR spectroscopy. Two-dimensional 1H-NMR spectra show that, in the presence of Ca2+, DAHPC binds to the active site of the enzyme in a similar manner to other phospholipid amide substrate analogs. The environment of the labeled carbonyl group has been investigated by a combination of 13C-NMR and difference-Fourier-transform IR spectroscopy. The carbonyl resonance shifts 3 ppm downfield on the binding of DAHPC to PLA2. The carbonyl absorption frequency decreases by 14-18 cm-1, accompanied by a marked sharpening of the absorption band. Thus, the carbonyl bond undergoes significant polarization in the enzyme-ligand complex, facilitated by the enzyme-bound Ca2+ ion. This suggests that ground-state strain is likely to promote catalysis in the case of substrate binding. Simple calcns. based on the IR data indicate that the carbonyl bond is weakened by 5-9 kJ/mol. This is the first reported observation of the amide vibration of a bound ligand against the strong background of protein amide vibrations.

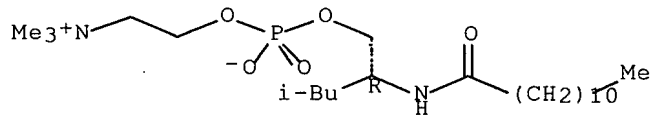
IT **145038-81-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and phospholipase A2 binding of)
RN 145038-81-9 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium-9-13C, 4-hydroxy-N,N,N-trimethyl-7-(2-methylpropyl)-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **131736-69-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and phospholipase A2 binding of, enzyme reaction mechanism in relation to)
RN 131736-69-1 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-7-(2-methylpropyl)-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



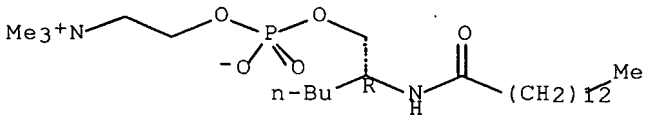
CC 7-3 (Enzymes)
Section cross-reference(s): 9
IT **145038-81-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and phospholipase A2 binding of)
IT **131736-69-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and phospholipase A2 binding of, enzyme reaction mechanism in relation to)

L49 ANSWER 24 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:546110 HCAPLUS Full-text
DOCUMENT NUMBER: 117:146110
TITLE: Competitive inhibition of lipolytic enzymes. VIII: Inhibitor-induced aggregation of porcine pancreatic phospholipase A2
AUTHOR(S): Deveer, A. M. T. J.; Den Ouden, A. T.; Vincent, M.; Gallay, J.; Verger, R.; Egmond, M. R.; Verheij, H. M.; De Haas, G. H.
CORPORATE SOURCE: Unilever Res. Lab., Vlaardingen, 3130 AC, Neth.
SOURCE: Biochimica et Biophysica Acta, Lipids and Lipid Metabolism (**1992**), 1126(1), 95-104
CODEN: BBLLA6; ISSN: 0005-2760
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Several 2-acylaminophospholipid analogs have previously been demonstrated to behave as potent competitive inhibitors of porcine pancreatic phospholipase A2 (I). Their inhibitory power appeared to be strictly controlled by the stereoconfiguration around the chiral C-2 atom and effective inhibition of the enzyme was observed only when incorporated into a micellar substrate-water interface. Here, various direct binding techniques were applied to investigate the interaction of the enzyme with pure micelles of the stereoisomeric forms of 2-tetradecanoylaminohexanol-1-phosphocholine (R-C14-PN and S-C14-PN). Upon equilibrium gel filtration of the enzyme (monomeric mol. weight = 14 kDa) on calibrated Superdex columns running in micellar solns. of R-C14-PN, I eluted as a lipid-protein complex of 74 kDa. Under identical conditions, micellar solns. of S-C14-PN did not give rise to high-mol.-weight aggregates and I eluted at its normal 14-kDa position. Light scattering expts., ultrasedimentation, and time-resolved fluorescence spectroscopy studies confirmed the formation of a high-mol.-weight aggregate between I and R-C14-PN micelles. The ultimate complex was shown to consist of 4 I mols. and .apprx.10 inhibitor mols. Using time-resolved fluorescence spectroscopy, the interaction was studied between the active site of I and R-C14-PN mols., both incorporated in an inert lipid matrix.

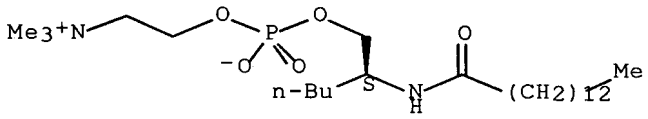
IT **131736-77-1**
RL: BIOL (Biological study)
(phospholipase A2 of pancreas aggregation induction by)
RN 131736-77-1 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphadocosan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



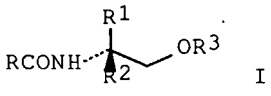
IT **143554-25-0**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(phospholipase A2 of pancreas response to)
RN 143554-25-0 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphadocosan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 7-5 (Enzymes)
IT **131736-77-1**
RL: BIOL (Biological study)
(phospholipase A2 of pancreas aggregation induction by)
IT **143554-25-0**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(phospholipase A2 of pancreas response to)

L49 ANSWER 25 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:511106 HCAPLUS Full-text
DOCUMENT NUMBER: 117:111106
TITLE: Design and synthesis of some substrate analog inhibitors of phospholipase A2 and investigations by NMR and molecular modeling into the binding interactions in the enzyme-inhibitor complex
AUTHOR(S): Bennion, Colin; Connolly, Stephen; Gensmantel, Nigel P.; Hallam, Catherine; Jackson, Clive G.; Primrose, William U.; Roberts, Gordon C. K.; Robinson, David H.; Slaich, Pritpal K.
CORPORATE SOURCE: Pharm. Div., Fisons PLC, Loughborough/Leicestershire, LE11 0RH, UK
SOURCE: Journal of Medicinal Chemistry (**1992**), 35(16), 2939-51
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:111106
GI

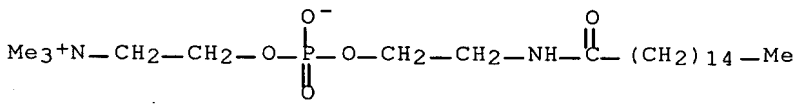


I

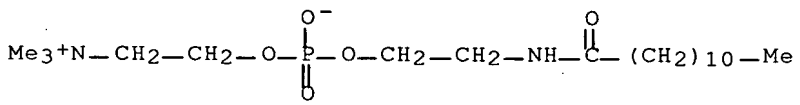
AB Phosphonoethyl amides I [R = Me(CH2)n, 2-C10H7, 2-C10H7CH2, (E)-Me(CH2)4CH:CHCH2CH2; R1 = H, Me, Me2CHCH2, PhCH2; R2 = H, Me2CHCH2; R3 = phosphocholine, PO(OH)OCH2CH2OH, PO(OH)2; n = 10, 14] were designed and prepared as substrate analog inhibitors of pancreatic phospholipase A2. I were tested in a novel dual-screening system based on parallel assays with monomeric and micellar substrates. Intermol. nuclear Overhauser effects between vinylic protons on one inhibitor and identified active site residues on the bovine pancreatic enzyme have been observed in solution NMR studies of the enzyme-inhibitor complex. It was deduced from both the biochem. results and the NMR data that the mode of interaction between this type of inhibitor and the active site of phospholipase A2 is essentially the same, irresp. of the presence or absence of an aggregated phospholipid surface. A model of the binding between the enzyme and inhibitor which incorporates the two-dimensional NMR data has been developed. The model can account for the activity of modified inhibitor structures and can be extrapolated to an assessment of the mode of binding of the natural substrate itself.

IT **76506-51-9P 82755-91-7P 142003-37-0P 142003-38-1P 142128-48-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and phospholipase A2 inhibitory activity of)

RN 76506-51-9 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphatetracosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide (9CI) (CA INDEX NAME)

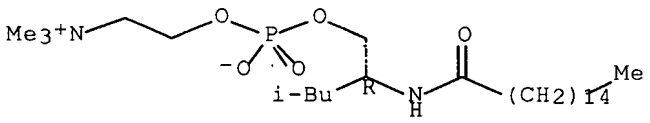


RN 82755-91-7 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



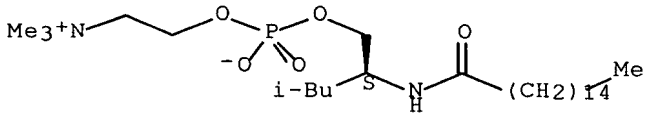
RN 142003-37-0 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphatetracosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-7-(2-methylpropyl)-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



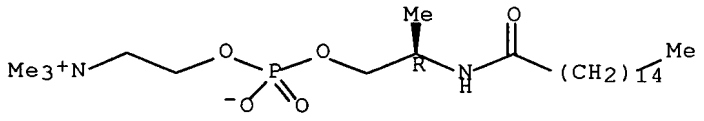
RN 142003-38-1 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphatetracosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-7-(2-methylpropyl)-9-oxo-, inner salt, 4-oxide, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 142128-48-1 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphatetracosan-1-aminium, 4-hydroxy-N,N,N,7-tetramethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI). (CA INDEX NAME)

Absolute stereochemistry.



CC 23-17 (Aliphatic Compounds)
Section cross-reference(s): 1, 7, 9
IT **76506-51-9P 82755-91-7P** 142003-33-6P
142003-34-7P **142003-37-0P 142003-38-1P**
142003-39-2P 142003-41-6P 142003-42-7P 142003-46-1P
142003-47-2P **142128-48-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and phospholipase A2 inhibitory activity of)

L49 ANSWER 26 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:465348 HCAPLUS Full-text
DOCUMENT NUMBER: 117:65348
TITLE: Competitive inhibition of lipolytic enzymes. VII. The interaction of pancreatic phospholipase A2 with micellar lipid/water interfaces of competitive inhibitors
AUTHOR(S): Deveer, A. M. T. J.; Franken, P. A.; Dijkman, R.; Meeldijk, J.; Egmond, M. R.; Verheij, H. M.; Verger, R.; De Haas, G. H.
CORPORATE SOURCE: Unilever Res., Vlaardingen, Neth.
SOURCE: Biochimica et Biophysica Acta, Lipids and Lipid Metabolism (**1992**), 1125(1), 73-81
CODEN: BBLLA6; ISSN: 0005-2760
DOCUMENT TYPE: Journal
LANGUAGE: English

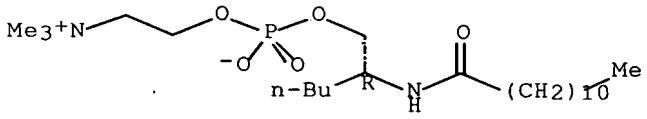
AB In a recent series of kinetic studies (De Haas G. H. et al., 1990) it was demonstrated that synthetic (R)-phospholipid analogs containing a 2-acylamino group, instead of the 2-acyloxy function found in natural phospholipids, behave as strong competitive inhibitors of porcine pancreatic phospholipase A2 (PLA2). It was also shown that these analogs strongly bind to the active site of the enzyme, but only after their incorporation into a micellar substrate/water interface. In the present study, an investigation was made of the interaction of native PLA2 and of an inactive PLA2, in which the active site residue His-48 has been modified by alkylation with 1-bromo-2-octanone, with pure micelles of several of these inhibitors in both enantiomeric forms by means of UV difference absorption spectroscopy. The results show that the first interaction step between native or modified enzyme and micellar lipid/water interfaces probably consists of a low-affinity Langmuir-type adsorption characterized by signals arising from the perturbation of the single Trp-3 residue. Once present at the interface the native enzyme is able to bind, in a second step, a single inhibitor mol. of the (R)-configuration in its active site, whereas the (S)-enantiomer is not bound in the active site. The overall dissociation constant of the interfacial phospholipase-inhibitor complex is 3 orders of magnitude lower for micelles composed of the (R)-isomer than those of the (S)-isomer. The modified PLA2 still adsorbs to micellar lipid/water interfaces but cannot bind either of the 2 enantiomers to its active site; similar dissociation consts. were found for lipid-protein complexes with micelles of either the (R) or the (S) inhibitors. After blanking the UV signals due to the perturbation of Trp-3 in the initial adsorption step of the enzyme to a micellar surface of a non-inhibitory phospholipid analog, the progressive binding of a single (R)-inhibitor mol. to the active site could be followed quant. by tyrosine perturbation. These titrns. yielded numerical values for the dissociation consts. in the interface and provide a possible explanation for the large difference in overall dissociation consts. of the complexes between enzyme and micelles of (R)-and (S)-inhibitors. With the use of PLA2 mutants in which each time a single tyrosine was replaced by phenylalanine, the tyrosine residues involved in binding of the monomeric inhibitor mol. were identified as Tyr-69 and Tyr-52.

IT **131736-68-0**
RL: BIOL (Biological study)
(phospholipase A2 of pancreas interaction with, at micelle interface, mechanism of, structure in relation to)

RN 131736-68-0 HCAPLUS

CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 7-3 (Enzymes)

IT **131736-68-0** 131736-78-2 142629-53-6 142629-54-7
RL: BIOL (Biological study)
(phospholipase A2 of pancreas interaction with, at micelle interface, mechanism of, structure in relation to)

L49 ANSWER 27 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:426980 HCAPLUS Full-text
DOCUMENT NUMBER: 117:26980
TITLE: Rapid synthesis of 2-desoxy-2-amino-3-phosphocholine-glycerinic-acid-alkylester,

1-alkyl-1-desoxy- and 1-O-alkyl-2-desoxy-2-amino-sn-glycero-3-phosphocholines, -3-phospho-N,N'-dimethylethanolamine and -3-phospho-Fmoc-serine-methylester

AUTHOR(S): Deigner, Hans Peter; Fyrnys, Beatrix

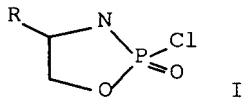
CORPORATE SOURCE: Pharm.-Chem. Inst., Univ. Heidelberg, Heidelberg, D-6900, Germany

SOURCE: Chemistry and Physics of Lipids (**1992**), 61(2), 199-208
CODEN: CPLIA4; ISSN: 0009-3084

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

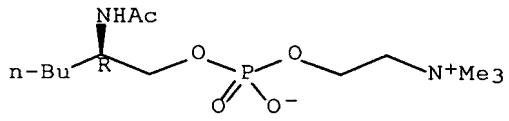
AB H2NCHRCH2OP(O)(O-)OCH2CH2N+Me3 [R = CO2(CH2)nMe, Bu, CH2O(CH2)pMe; n = 4, 7; p = 7, 9] were prepared from the alcs. H2NCHRCH2OH by cyclization with POCl3, reaction of the oxaazaphospholanes I with choline tosylate, and hydrolysis. Me(CH2)9OCH2CH(NH2)CH2OP(O)(OH)OC H2CH2NMe2 and Me(CH2)9OCH2CH(NH2)CH2OP(O)(OH)OCH2CH(NHR1)CO2Me (R1 = 9-fluorenylmethoxycarbonyl) were similarly prepared

IT **141858-56-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 141858-56-2 HCAPLUS

CN 3,5-Dioxa-8-aza-4-phosphadecan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 33-6 (Carbohydrates)

IT 141858-54-0P 141858-55-1P **141858-56-2P** 141858-57-3P
141858-58-4P 141858-62-0P 141858-64-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L49 ANSWER 28 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1992:207317 HCAPLUS Full-text

DOCUMENT NUMBER: 116:207317

TITLE: Competitive inhibition of lipolytic enzymes. VI. Inhibition of two human phospholipases A2 by acylamino phospholipid analogs

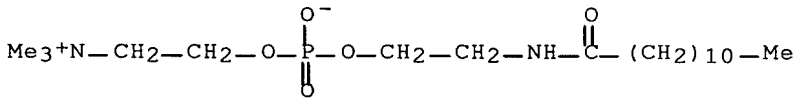
AUTHOR(S): Van den Berg, L.; Franken, P. A.; Verheij, H. M.; Dijkman, R.; De Haas, G. H.

CORPORATE SOURCE: Dep. Enzymol. Protein Eng., State Univ. Utrecht, Utrecht, 3584 CH, Neth.
SOURCE: Biochimica et Biophysica Acta, Lipids and Lipid Metabolism (**1992**), 1124(1), 66-70
CODEN: BBLLA6; ISSN: 0005-2760
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The competitive inhibition of human pancreatic and a mutant human platelet phospholipase A2 (PLA2) was investigated using acylamino phospholipid analogs, which are potent competitive inhibitors of porcine pancreatic PLA2. Both the mutant platelet PLA2 and the human pancreatic PLA2 are effectively inhibited by these compds. The enzyme from platelets is most strongly inhibited by compds. with a neg. charged phosphoglycol headgroup. Compds. with a neutral phosphocholine headgroup are only weak inhibitors, whereas an inhibitor with a phosphoethanolamine headgroup shows an intermediate inhibitory capacity. The platelet PLA2 is most effectively inhibited by neg. charged inhibitors having a relatively short (four or more carbon atoms) alkylchain on position one and a acylamino chain of 14 carbon atoms on position two. For the pancreatic enzyme an inhibitor with a phosphoethanolamine headgroup was more effective than inhibitors with either a phosphocholine or a phosphoglycol headgroup. The chain length preference of the pancreatic enzyme resembles that of the platelet PLA2. The largest discrimination in inhibition between the human platelet and the human pancreatic PLA2 is obtained with inhibitors with a neg. charged phosphoglycol headgroup, an alkyl chain of four carbon atoms on position one and a long acylamino chain of 14-16 carbon atoms on position two. Because the platelet PLA2 is though to have several biol. functions, specific inhibitors of this enzyme could have important implications in the design of pharmaceutically interesting compds.

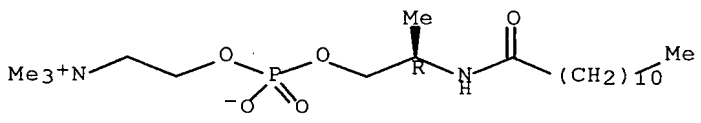
IT **82755-91-7 131736-65-7 131736-66-8 131736-68-0 131736-71-5 131736-73-7 131736-75-9 131736-76-0 131736-77-1 131736-79-3 131764-77-7**
RL: BIOL (Biological study)
(phospholipase A2 of human pancreas and platelet inhibition by, structure in relation to)

RN 82755-91-7 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



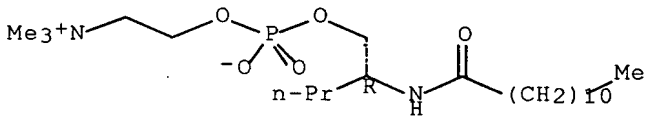
RN 131736-65-7 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 4-hydroxy-N,N,N,7-tetramethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



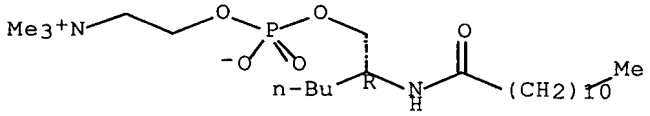
RN 131736-66-8 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-9-oxo-7-propyl-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



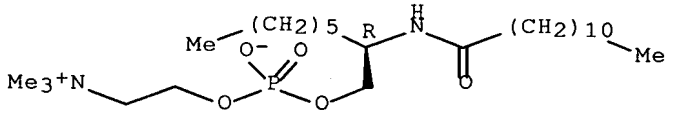
RN 131736-68-0 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



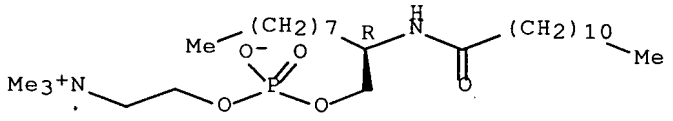
RN 131736-71-5 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 7-hexyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



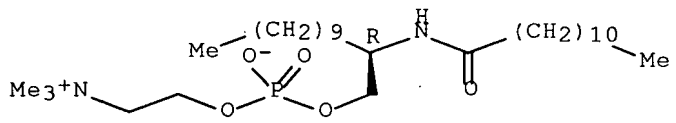
RN 131736-73-7 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-7-octyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



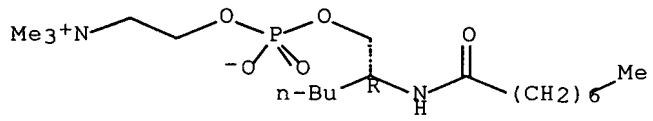
RN 131736-75-9 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 7-decyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



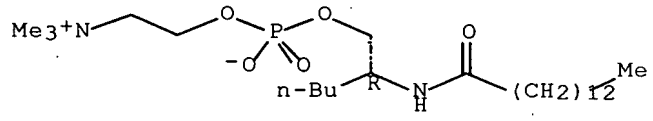
RN 131736-76-0 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphahexadecan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



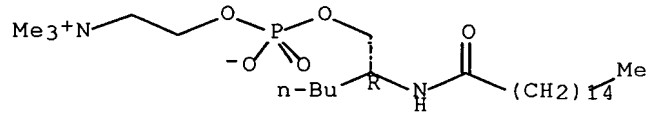
RN 131736-77-1 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphadocosan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



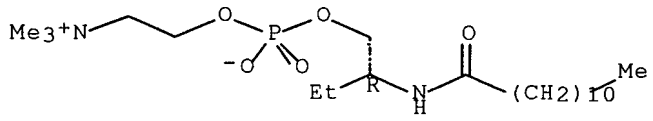
RN 131736-79-3 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphatetracosan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



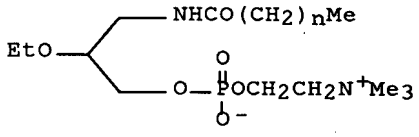
RN 131764-77-7 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 7-ethyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 1-3 (Pharmacology)
Section cross-reference(s): 7
IT **82755-91-7** 127612-62-8 131736-59-9 131736-63-5
131736-65-7 **131736-66-8** **131736-68-0**
131736-71-5 **131736-73-7** **131736-75-9**
131736-76-0 **131736-77-1** 131736-78-2
131736-79-3 131736-80-6 **131764-77-7**
131764-78-8 136134-09-3 141056-42-0 141056-43-1 141056-44-2
141056-45-3 141056-46-4 141056-47-5
RL: BIOL (Biological study)
(phospholipase A2 of human pancreas and platelet inhibition by, structure in relation to)

L49 ANSWER 29 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1991:185881 HCAPLUS Full-text
DOCUMENT NUMBER: 114:185881
TITLE: In vitro evaluation of phosphocholine and quaternary ammonium containing lipids as novel anti-HIV agents
AUTHOR(S): Meyer, Karen L.; Marasco, Canino J., Jr.; Morris-Natschke, Susan L.; Ishaq, Khalid S.; Piantadosi, Claude; Kucera, Louis S.
CORPORATE SOURCE: Sch. Pharm., Univ. North Carolina, Chapel Hill, NC, 27599, USA
SOURCE: Journal of Medicinal Chemistry (**1991**), 34(4), 1377-83
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 114:185881
GI



I

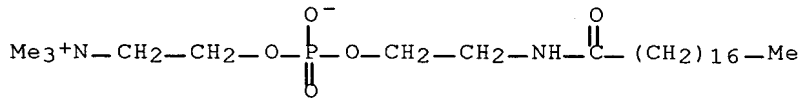
AB A series of synthetic lipids containing a two- or three-carbon backbone substituted with a thio, oxy, or amidoalkyl functionality and either a phosphocholine or quaternary ammonium moiety were evaluated as potential anti-HIV-1 agents. Several analogs were identified as possessing activity with the most promising compound being rac-3-octadecanamido-2-ethoxypropylphosphocholine (I). I exhibited an IC50 for the inhibition of plaque formation of 0.16 μM which was 84-fold lower than the IC50 value determined for CEM-SS cell growth inhibition. Initial mechanistic studies have indicated that these compds., unlike AZT, are not reverse transcriptase (RT) inhibitors, but instead appear to inhibit a late step in HIV replication involving virus assembly and infectious virus production Since

these lipids are acting via a different, mechanism they represent an alternative approach to the chemotherapeutic treatment of AIDS as well as candidates for combination therapy with AZT.

IT **82755-92-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and anti-HIV-1 activity of)

RN 82755-92-8 HCAPLUS

CN 3,5-Dioxa-8-aza-4-phosphahexacosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



CC 33-7 (Carbohydrates)
Section cross-reference(s): 1

IT **82755-92-8P** 128723-54-6P 131933-54-5P 131933-56-7P 131933-64-7P 149576-19-2P 149576-20-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and anti-HIV-1 activity of)

L49 ANSWER 30 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1991:77532 HCAPLUS Full-text

DOCUMENT NUMBER: 114:77532

TITLE: Competitive inhibition of lipolytic enzymes. IV. Structural details of acylamino phospholipid analogs important for the potent inhibitory effects on pancreatic phospholipase A2

AUTHOR(S): De Haas, G. H.; Dijkman, R.; Ransac, S.; Verger, R.

CORPORATE SOURCE: Lab. Biochem., CBLE, Utrecht, 3584 CH, Neth.

SOURCE: Biochimica et Biophysica Acta, Lipids and Lipid Metabolism (**1990**), 1046(3), 249-57
CODEN: BBLLA6; ISSN: 0005-2760

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 1-Acyl-2(R)-acylamino phospholipids are effective competitive inhibitors of porcine pancreatic phospholipase A2 (EC 3.1.1.4). By systematically varying the substituent at C-1 and the acyl chain length at C-2, a series of phospholipid analogs was obtained for which the inhibitory power was determined in a detergent-containing and occasionally also in a detergent-free micellar substrate system. The recently proposed kinetic model applicable to water-insol. inhibitors allowed a quant. comparison of the inhibitory power Z of the various substrate analogs. Using as substrate (R)-1,2-didodecanoylglycero-3-phosphocholine in mixed micelles with Na taurodeoxycholate, an inhibitor mol. showed a Z value of 15,000. This implies an affinity of the inhibitor for the active site of the enzyme >4-orders of magnitude stronger as compared with the substrate mol. Slightly longer and shorter 1-acyl chain lengths resulted in a sharp drop of the inhibitory power, which suggests that the enzyme must possess a rather short, but well-defined hydrophobic binding pocket for the C-1 alkyl chain. Variation of the 2-acylamino group length (n) resulted in inhibitors with nearly equal Z-values for n - 11, 13 and 15. Most probably the binding cleft on the enzyme for the C-2 acylamino chain is longer, more loosely constructed and contributing less to the overall binding energy. Several members of the 2-acylamino phospholipids are water-soluble and possess relatively high critical micelle concns. Their inhibitory power could be

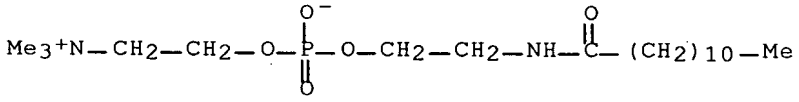
tested not only in micellar substrate dispersions but also in assay systems where both the inhibitor and substrate are molecularly dispersed. It appeared that these water-soluble phospholipid analogs are effective inhibitors of the enzyme only after incorporation into an organized substrate/water interface. In contrast, in molecularly dispersed substrate solns. the same mols. have completely lost their inhibitory power. These observations support the kinetic model of lipolysis and interfacial inhibition.

IT **82755-91-7 131736-65-7 131736-66-8 131736-67-9 131736-68-0 131736-69-1 131736-70-4 131736-71-5 131736-72-6 131736-73-7 131736-74-8 131736-75-9 131736-76-0 131736-77-1 131736-79-3 131764-77-7**

RL: BIOL (Biological study)
(phospholipase A2 of pancreas inhibition by, structure in relation to)

RN 82755-91-7 HCAPLUS

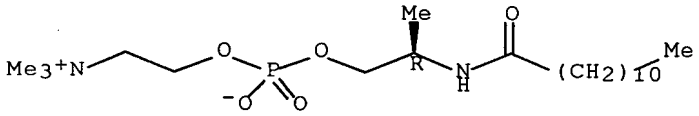
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



RN 131736-65-7 HCAPLUS

CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 4-hydroxy-N,N,N,7-tetramethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

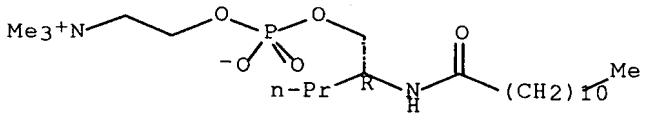
Absolute stereochemistry.



RN 131736-66-8 HCAPLUS

CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-9-oxo-7-propyl-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

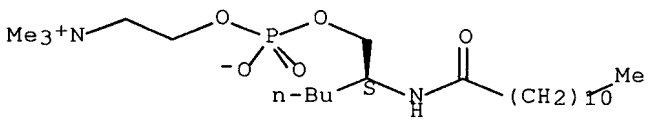
Absolute stereochemistry.



RN 131736-67-9 HCAPLUS

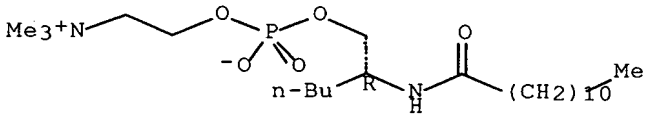
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



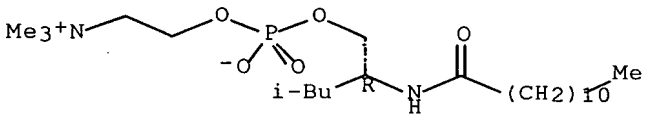
RN 131736-68-0 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



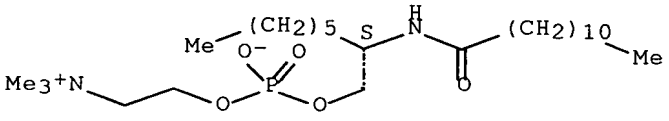
RN 131736-69-1 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-7-(2-methylpropyl)-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



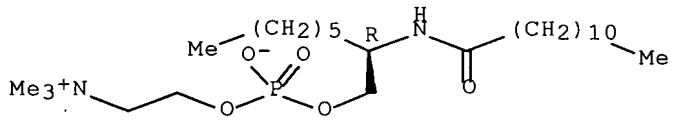
RN 131736-70-4 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 7-hexyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



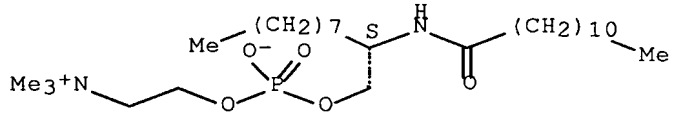
RN 131736-71-5 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 7-hexyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



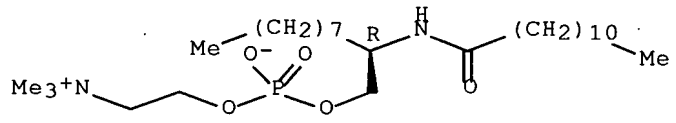
RN 131736-72-6 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-7-octyl-9-oxo-, inner salt, 4-oxide, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



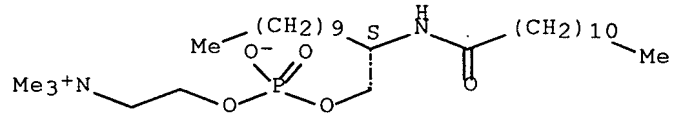
RN 131736-73-7 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-7-octyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



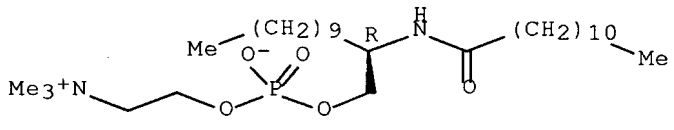
RN 131736-74-8 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 7-decyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



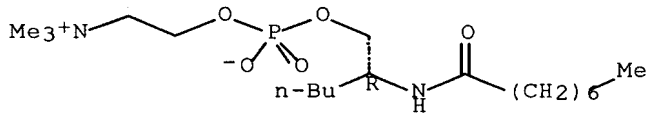
RN 131736-75-9 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 7-decyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



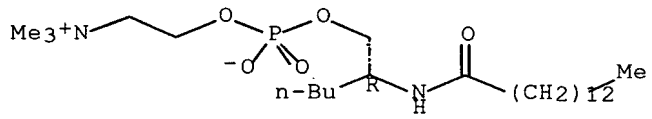
RN 131736-76-0 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphahexadecan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



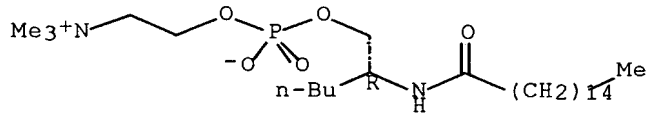
RN 131736-77-1 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphadocosan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



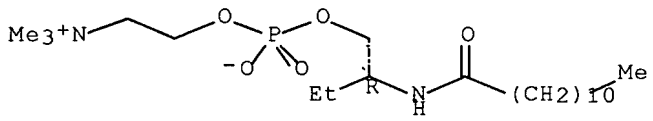
RN 131736-79-3 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphatetracosan-1-aminium, 7-butyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 131764-77-7 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 7-ethyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 7-3 (Enzymes)
IT **82755-91-7** 127612-62-8 131736-55-5 131736-56-6
131736-57-7 131736-58-8 131736-59-9 131736-60-2 131736-61-3
131736-62-4 131736-63-5 131736-64-6 **131736-65-7**
131736-66-8 131736-67-9 131736-68-0
131736-69-1 131736-70-4 131736-71-5
131736-72-6 131736-73-7 131736-74-8
131736-75-9 131736-76-0 131736-77-1
131736-78-2 **131736-79-3** 131736-80-6 **131764-77-7**
131764-78-8 131830-81-4
RL: BIOL (Biological study)
(phospholipase A2 of pancreas inhibition by, structure in relation to)

L49 ANSWER 31 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1987:149474 HCAPLUS Full-text
DOCUMENT NUMBER: 106:149474
TITLE: Phospholipid analogs useful as platelet-activating factor synthesis inhibitors, their preparation, and pharmaceutical compositions containing them
INVENTOR(S): Bugianesi, Robert L.; Ponpipom, Mitree M.; Rupprecht, Kathleen M.
PATENT ASSIGNEE(S): Merck and Co., Inc. , USA
SOURCE: Eur. Pat. Appl., 59 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

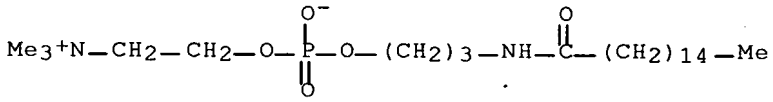
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 208961	A2	19870121	EP 1986-108693	19860626
			<--	
EP 208961	A3	19880420		
R: CH, DE, FR, GB, IT, LI, NL				
US 4761404	A	19880802	US 1985-750435	19850701
			<--	
JP 62012754	A	19870121	JP 1986-152847	19860701
			<--	
PRIORITY APPLN. INFO.:			US 1985-750435 A	19850701
			<--	

OTHER SOURCE(S): MARPAT 106:149474

AB Phospholipid analogs RYCHR2(CH2)mCHR3Z(CH2)nX [R = saturated or unsatd. C12-20 alkyl, substituted aralkyl or heteroaralkyl, cholesteryl; Y = O, NHCO, NHCO2, NHSO2, NHCONH; R2, R3 = H, OH, (substituted) C1-4 alkyl, N3, AcNH, etc.; Z = OP(O)(OH)O, CH2P(O)(OH)O, CH2P(O)(OH)CH2, CH2SOCH2, CH2SO2CH2; X = N+Me3, alkoxy, alkoxycarbonylamino, OH, F, N3, NH2, cyano, etc.; m = 0-4; n = 2-6] are prepared as inhibitors of platelet-activating factor (PAF) formation which are useful for treatment of PAF-mediated diseases. C16H33OCH2CH(OH)CH2OCPh3 was converted by successive treatment with CrO3/pyridine, MeLi, 2-chloro-2-oxo-1,3,2-dioxophosphorane, and NMe3 to C16H33OCH2CMe(OH)CH2OP(O)(OH)OCH2CH2N+Me3. This compound at 10 μM caused 73% inhibition of PAF biosynthesis in vitro, measured by the procedure of Wykle, et al. (1980).

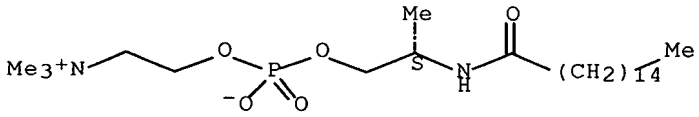
IT **76506-52-0P 76506-59-7P 76549-57-0P 107560-80-5P 107560-81-6P 107655-53-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as blood platelet-activating factor formation inhibitor)

RN 76506-52-0 HCAPLUS
CN 3,5-Dioxa-9-aza-4-phosphapentacosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-10-oxo-, inner salt, 4-oxide (9CI) (CA INDEX NAME)

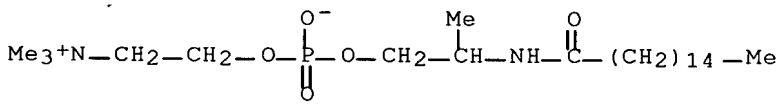


RN 76506-59-7 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphatetracosan-1-aminium, 4-hydroxy-N,N,N,7-tetramethyl-9-oxo-, inner salt, 4-oxide, (S)- (9CI) (CA INDEX NAME)

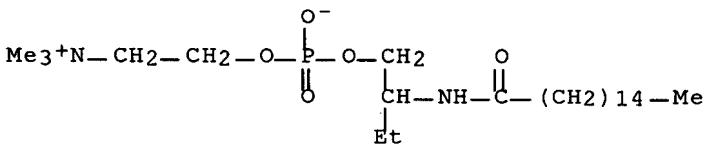
Absolute stereochemistry.



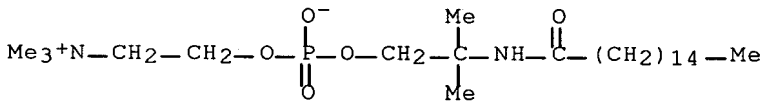
RN 76549-57-0 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphatetracosan-1-aminium, 4-hydroxy-N,N,N,7-tetramethyl-9-oxo-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



RN 107560-80-5 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphatetracosan-1-aminium, 7-ethyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide (9CI) (CA INDEX NAME)

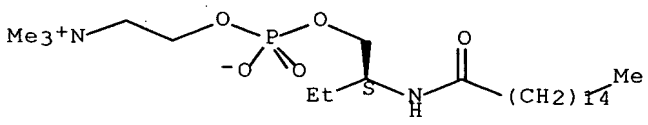


RN 107560-81-6 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphatetracosan-1-aminium, 4-hydroxy-N,N,N,7,7-pentamethyl-9-oxo-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



RN 107655-53-8 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphatetracosan-1-aminium, 7-ethyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide, (S)- (9CI) (CA INDEX NAME)

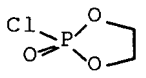
Absolute stereochemistry.

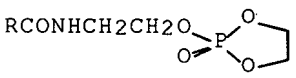


IC ICM C07F009-10
ICS C07F009-09; A61K031-66
CC 1-7 (Pharmacology)
Section cross-reference(s): 23
IT **76506-52-0P 76506-59-7P 76549-57-0P**
107560-67-8P 107560-68-9P 107560-69-0P 107560-70-3P
107560-71-4P 107560-72-5P 107560-73-6P 107560-79-2P
107560-80-5P 107560-81-6P 107560-82-7P
107560-83-8P 107560-84-9P 107560-85-0P 107560-86-1P
107560-87-2P 107560-88-3P 107560-89-4P 107560-90-7P
107560-91-8P 107560-92-9P 107560-93-0P 107560-95-2P
107560-96-3P 107560-97-4P 107560-98-5P 107560-99-6P
107655-53-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as blood platelet-activating factor formation inhibitor)

L49 ANSWER 32 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1982:492712 HCAPLUS Full-text
DOCUMENT NUMBER: 97:92712
TITLE: Synthesis of enzyme-inhibitory phospholipid analogs. III. A facile synthesis of N-acylaminoethylphosphorylcholines
AUTHOR(S): Chandrakumar, Nizal S.; Boyd, Victoria L.; Hajdu, Joseph

CORPORATE SOURCE: Dep. Chem., Boston Coll., Chestnut Hill, MA, 02167, USA
SOURCE: Biochimica et Biophysica Acta, Lipids and Lipid Metabolism (**1982**), 711(2), 357-60
CODEN: BBLLA6; ISSN: 0005-2760
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

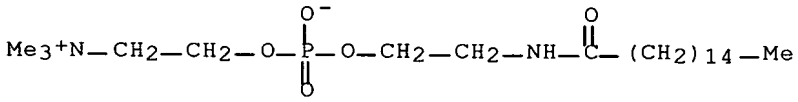

II


III

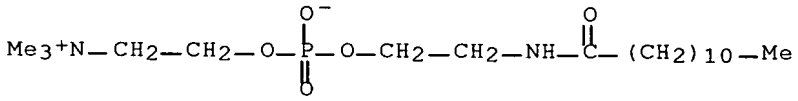
AB Title cholines RCONHCH2CH2OP(O)(O-)OCH2CH2N+Me3 (I; RCO = lauroyl, palmitoyl, stearoyl) were prepared by acylating H2NCH2CH2OH with RCOCl, treating the resulting RCONHCH2CH2OH with phospholane II, and cleaving the ring of the resulting cyclic phosphates III with Me3N. I are phospholipase A2 inhibitors.

IT **76506-51-9P 82755-91-7P 82755-92-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as phospholipase A2 inhibitor)

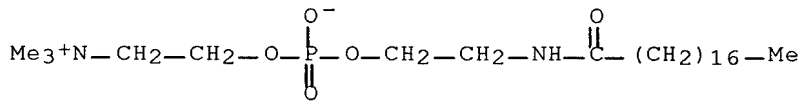
RN 76506-51-9 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphatetracosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



RN 82755-91-7 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphaeicosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



RN 82755-92-8 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphahexacosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



CC 34-2 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 7

IT **76506-51-9P 82755-91-7P 82755-92-8P**
82755-93-9DP, N-fatty acyl derivs.
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as phospholipase A2 inhibitor)

L49 ANSWER 33 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1981:83634 HCAPLUS Full-text
DOCUMENT NUMBER: 94:83634
TITLE: Phosphorylcholines
PATENT ASSIGNEE(S): Toyama Chemical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 27 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 55118494	A	19800911	JP 1979-25643	19790307
			<--	
JP 62052757	B	19871106		
PRIORITY APPLN. INFO.:			JP 1979-25643 A	19790307
			<--	

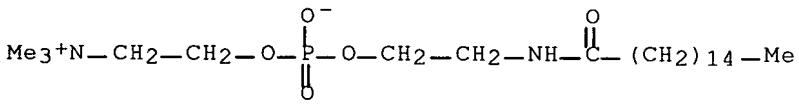
AB Twenty-nine phosphorylcholines, useful as antitumor agents (data given in mice against Ehrlich ascites and Sarcoma 180 tumor cells), were prepared Thus, stirring 10 g 2-(N-palmitoylamino)ethanol in THF with 13.5 g Et3N and 8.9 g 2-bromoethyl phosphorodichloridate at 0-5° and stirring 2 h at room temperature gave an oil, which was stirred with aqueous CHCl3 2 h at 0-5°, made pH 2.5, and the resulting organic layer concentrated, and autoclaved with 10 mL Me3N in MeCOEt 10 h at 55-60° to give 1.2 g 2-(N-palmitoylamin)ethyl 2-trimethylammonioethyl phosphate bromide (I). Stirring 1 g I with 0.4 g AgOAc in MeOH 3 h at room temperature and keeping overnight gave 0.6 g 2-(N-palmitoylamino)ethyl 2-trimethylammonioethyl phosphate.

IT **76506-51-9P 76506-52-0P 76506-53-1P**
76506-59-7P 76506-60-0P 76506-63-3P
76506-65-5P 76506-68-8P 76506-69-9P
76506-70-2P 76506-73-5P 76506-75-7P
76523-45-0P 76523-46-1P 76549-57-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and anticancer activity of)

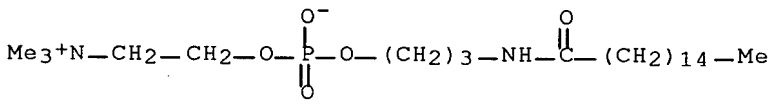
RN 76506-51-9 HCAPLUS

CN 3,5-Dioxa-8-aza-4-phosphatetracosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



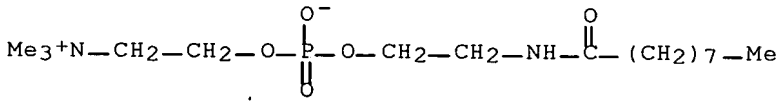
RN 76506-52-0 HCAPLUS

CN 3,5-Dioxa-9-aza-4-phosphapentacosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-10-oxo-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



RN 76506-53-1 HCAPLUS

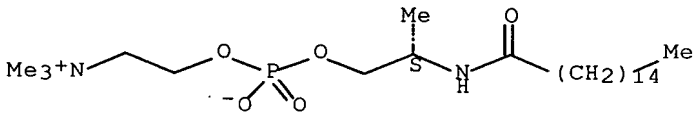
CN 3,5-Dioxa-8-aza-4-phosphaheptadecan-1-aminium, 4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



RN 76506-59-7 HCAPLUS

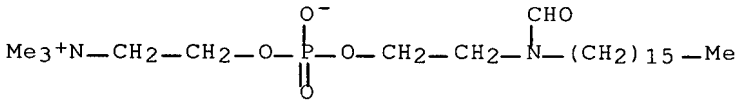
CN 3,5-Dioxa-8-aza-4-phosphatetracosan-1-aminium, 4-hydroxy-N,N,N,7-tetramethyl-9-oxo-, inner salt, 4-oxide, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

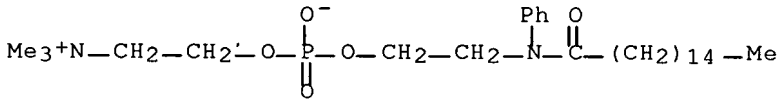


RN 76506-60-0 HCAPLUS

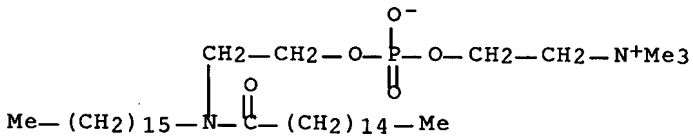
CN 3,5-Dioxa-8-aza-4-phosphatetracosan-1-aminium, 8-formyl-4-hydroxy-N,N,N-trimethyl-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



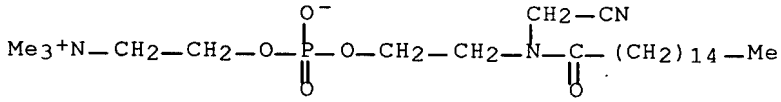
RN 76506-63-3 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphatetracosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-9-oxo-8-phenyl-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



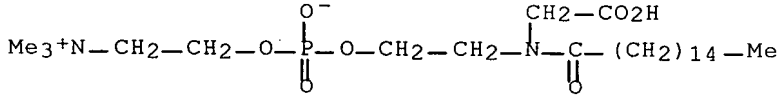
RN 76506-65-5 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphatetracosan-1-aminium, 8-hexadecyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



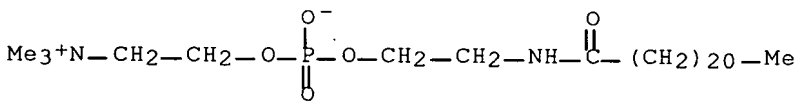
RN 76506-68-8 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphatetracosan-1-aminium, 8-(cyanomethyl)-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



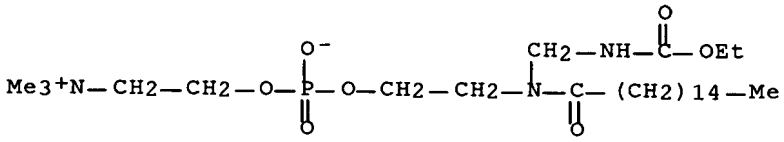
RN 76506-69-9 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphatetracosan-1-aminium, 8-(carboxymethyl)-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



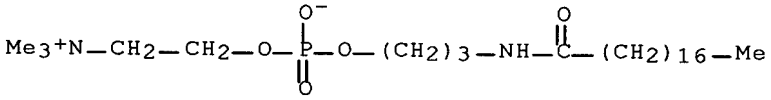
RN 76506-70-2 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphatriacontan-1-aminium, 4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



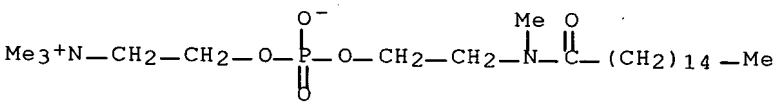
RN 76506-73-5 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphatetracosan-1-aminium, 8-[[(ethoxycarbonyl)amino]methyl]-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



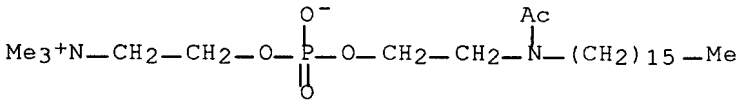
RN 76506-75-7 HCAPLUS
CN 3,5-Dioxa-9-aza-4-phosphaheptacosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-10-oxo-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



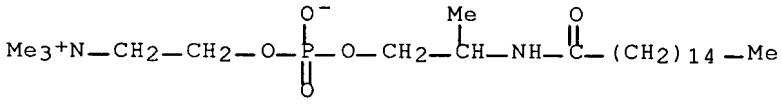
RN 76523-45-0 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphatetracosan-1-aminium, 4-hydroxy-N,N,N,8-tetramethyl-9-oxo-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



RN 76523-46-1 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphatetracosan-1-aminium, 8-acetyl-4-hydroxy-N,N,N-trimethyl-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



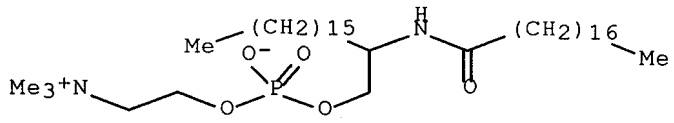
RN 76549-57-0 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphatetracosan-1-aminium, 4-hydroxy-N,N,N,7-tetramethyl-9-oxo-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



IC C07F009-06; A61K031-66
CC 23-18 (Aliphatic Compounds)
Section cross-reference(s): 63
IT **76506-51-9P 76506-52-0P 76506-53-1P**
76506-54-2P 76506-55-3P 76506-56-4P 76506-57-5P 76506-58-6P
76506-59-7P 76506-60-0P 76506-61-1P
76506-62-2P **76506-63-3P** 76506-64-4P **76506-65-5P**
76506-66-6P 76506-67-7P **76506-68-8P 76506-69-9P**
76506-70-2P 76506-71-3P 76506-72-4P **76506-73-5P**
76506-74-6P **76506-75-7P** 76506-76-8P **76523-45-0P**
76523-46-1P 76549-57-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and anticancer activity of)

L49 ANSWER 34 OF 34 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:30322 HCAPLUS Full-text
DOCUMENT NUMBER: 84:30322
TITLE: Synthesis of 3-deoxysphingomyelin
AUTHOR(S): Orlova, E. G.; Mitsner, B. I.; Zvonkova, E. N.; Evstigneeva, R. P.
CORPORATE SOURCE: Mosk. Inst. Tonkoi Khim. Tekhnol. im. Lomonosova, Moscow, USSR
SOURCE: Zhurnal Organicheskoi Khimii (**1975**), 11(9), 1821-5
CODEN: ZORKAE; ISSN: 0514-7492
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB (R = n-C16H33 in this abstract). Benzyloxycarbonylation of H2NCHRCH2OH yielded 97.8% PhCH2O2CNHCHRCH2OH, which was treated with Cl2P(O)OCH2CH2Cl at -10° to give 89.58% PhCH2O2CNHCHRCH2OP(O)(OH)OCH2CH2Cl (I) after acidic hydrolysis; hydrogenation of I and acylation with RCH2COCl gave 54.1% RCH2CONHCHRCH2OP(O)(OH)OCH2CH2Cl, which alkylated Me3N to give the title compound Alkylation of Me3N with I, followed by hydrogenation and acylation with RCH2COCl also yielded the title compound
IT **57785-10-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 57785-10-1 HCAPLUS
CN 3,5-Dioxa-8-aza-4-phosphahexacosan-1-aminium, 7-hexadecyl-4-hydroxy-N,N,N-trimethyl-9-oxo-, inner salt, 4-oxide (9CI) (CA INDEX NAME)



CC 23-8 (Aliphatic Compounds)
IT **57785-10-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

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